UNITED STATES
ENVIRONMENTAL PROTECTION AGENCY (EPA)
HIGH PRODUCTION VOLUME (HPV)
CHEMICAL CHALLENGE PROGRAM

ROBUST SUMMARIES DOSSIER
for MEMBERS of the
HIGHER OLEFINS CATEGORY
CONTAINING C11 to C13 OLEFINS

Members containing C11 – C13 olefins:
CAS No. 25378-22-7, Dodecene
CAS No. 2437-56-1, 1-Tridecene
CAS No. 68855-58-3Alkenes, C10-16 alpha
CAS No. 68526-57-8; Alkenes, C10-12, C11-Rich
CAS No. 68526-58-9; Alkenes, C11-13, C12-Rich
CAS No. 68783-10-8, Heavy polymerization naphtha (petroleum)
CAS No. 68991-52-6; Alkenes, C10-16
CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons
CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons
[Note: CAS No. 68526-56-7; Alkenes, C9-11, C10-rich is included in the C10 dossier]

Contains Robust Summaries for the Following Substances:
CAS No. 28761-27-5, Undecene (mixture of isomers)
CAS No. 112-41-4, 1-Dodecene
CAS No. 25378-22-7, Dodecene
CAS No. 2437-56-1, 1-Tridecene
CAS No. 25377-82-6, Tridecene
CAS No. 68526-57-8; Alkenes, C10-12, C11-Rich
CAS No. 68526-58-9; Alkenes, C11-13, C12-Rich
CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons
CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons
CAS No. 85535-87-1, Alkenes C10-13
C10-13 Internal olefins (SHOP Olefins 103PQ11/Olefins 103 PQ11/SHOP Olefins 103)
[see other dossiers for robust summaries for C10 and C14-C16 components of category members]

Prepared by:

American Chemistry Council
Higher Olefins Panel
April 28, 2005

1. GENERAL INFORMATION

1.01 Details on Chemical Category

The Higher Olefins Category consists of a non-continuous range of odd- and even-numbered mono-unsaturated linear and branched olefins (C_6 through C_{54}) under 30 CAS numbers, 13 for alpha olefins and 17 for internal olefins. All CAS numbers are within the HPV Challenge Program. The $C_6 - C_{14}$ even-numbered linear alpha olefins were sponsored under the OECD SIDS program (SIAM 11). The Panel sponsored the C_6, C_7, C_8, C_9, C_{10}, C_{12} and C_{10-13} aliphatic linear and branched internal olefins and the C_{16} and C_{18} aliphatic linear alpha olefins in the OECD HPV Chemicals Programme (SIAM 19). The members of the category are presented below.

Members of the Higher Olefins Category

Alpha Olefins	Branched/Linear	CAS No.
Neohexene	Branched	558-37-2
1-Tridecene	Linear	2437-56-1
1-Hexadecene (ICCA)	Linear	629-73-2
1-Octadecene (ICCA)	Linear	112-88-9
1-Eicosene	Linear	3452-07-1
1-Docosene	Linear	1599-67-3
1-Tetracosene	Linear	10192-32-2
Alkenes, C10-16 alpha	Linear	68855-58-3
Alkenes, C14-18 alpha	Linear	68855-59-4
Alkenes, C14-20 alpha	Linear	68855-60-7
a-Olefin fraction C20-24 cut	Linear	93924-10-8
a-Olefin fraction C24-28 cut	Branched and Linear	93924-11-9
Alkene, C24-54 branched and linear, alpha	Branched and Linear	131459-42-2
Internal Olefins		
Hexene (ICCA)	Linear	25264-93-1
Heptene (ICCA)	Linear	25339-56-4
Octene (ICCA)	Linear	25377-83-7
Nonene (ICCA)	Linear	27215-95-8
Dodecene (ICCA – not sponsored in HPV)	Linear	25378-22-7
Alkenes, C6	Branched and Linear	68526-52-3
Alkenes, C6-8, C7 rich	no data available	68526-53-4
Alkenes, C7-9, C8-rich	Linear	68526-54-5
Alkenes, C8-10, C9-rich	Linear	68526-55-6
Alkenes, C9-11, C10-rich	Linear	68526-56-7
Alkenes, C10-12, C11-rich	Linear	68526-57-8
Alkenes, C11-13, C12-rich	Linear	68526-58-9
Heavy polymerization naphtha (petroleum)	Branched	68783-10-8
Alkenes, C10-16	Linear	68991-52-6
Alkenes, C15-C18	Linear	93762-80-2
C10,12 Olefin rich hydrocarbons	Linear	68514-32-9
C12,14 Olefin rich hydrocarbons	Linear	68514-33-0

1.1 General Substance Information

A. Type of Substance

Element [ ]; Inorganic [ ]; Natural substance [ ]; Organic [X]; Organometallic [ ]; Petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

Gaseous [ ]; Liquid [X]; Solid [ ]

C. Purity: C11, C12 and/or C13 containing category members are manufactured and marketed as blends. 1-Tridecene is also manufactured and marketed as a pure product (90% or 100%).

1.2 Impurities

Remark: The compositions reported by manufacturers for the members of the Higher Olefins Category containing C11-C13 olefins are shown below:

Alpha Olefins	CAS No.	Composition/Impurities
1-Tridecene	2437-56-1	C13 linear. No impurities or branching; Also reported: C12 and lower olefins = 4% max., C13 = 90% min., C14 and higher olefins = 10% max., with max. 8% branched
Alkenes, C10-16 alpha	68855-58-3	Typical composition: 0.6% C10, 64.2% C12, 34.7% C14, 0.5% C16; 99.6% monoolefin; 0.4% paraffin; 86.5% linear terminal; 10.6% branched terminal; 2.9% linear internal
Internal Olefins		
Dodecene (ICCA – not sponsored in HPV)	25378-22-7	C10-13 internal olefin blend: Typical composition = <0.1% C_9 or lower, 11.2% C_{10}, 29.6% C_{11}, 25.9% C_{12}, 23.6% C_{13}, 9.5% C_{14} and 0.1 % >C_{14}; with 4.2% N-paraffins and 4.6% dienes as impurities
Alkenes, C10-12, C11-rich	68526-57-8	Typical composition: 1% C9 olefins, 10% C10 olefins, 76% C11 olefins, 13% C12 olefins. Also reported: Mostly linear, less than 2% branched.
Alkenes, C11-13, C12-rich	68526-58-9	Mostly linear, less than 2% branched.
Heavy polymerization naphtha	68783-10-8	Branched, C11-13, C12-rich olefins

(petroleum)		
Alkenes, C10-16	68991-52-6	Mostly linear, less than 2% branched.
C10,12 Olefin rich hydrocarbons	68514-32-9	0-1% C8, 10-30% C10, 70-90% C12, 0-1% C14, 0-50% paraffins
C12,14 Olefin rich hydrocarbons	68514-33-0	0-8% C12 and lower, 92-100% C14, 0-0.2% C16, 0-1% C14, 0-50% paraffins

1.3 Additives

None

1.4 Synonyms

1.5 Quantity

Remarks: A Chemical Economics Handbook marketing report indicated that 2000 global production for dodecene was approximately 695 million pounds (315,000 metric tons) with the United States accounting for 47% (SRI, 2001). U.S. production volumes for C11, C12 and C13 containing members of the Higher Olefins Category reported for 2002 by members of the American Chemistry Council's Higher Olefins Panel are shown below:

COMPOUND	CAS NUMBER	2002 U.S. PRODUCTION VOLUME (Million Pounds)
Alpha Olefins		
1-Tridecene	2437-56-1	1-10
Alkenes, C10-16 alpha	68855-58-3	1-10
Internal Olefins		
Dodecene (ICCA – not sponsored in HPV)	25378-22-7	1-10
Alkenes, C10-12, C11-rich	68526-57-8	50-100
Alkenes, C11-13, C12-rich	68526-58-9	100-200
Heavy polymerization naphtha	68783-10-8	50-100
Alkenes, C10-16	68991-52-6	400-500
C10,12 Olefin rich hydrocarbons	68514-32-9	1-10
C12,14 Olefin rich hydrocarbons	68514-33-0	1-10

Reference: American Chemistry Council's Higher Olefins Panel (2002)

1.6 Use Pattern

A. General Use Pattern

Type of Use:	Category:
(a) Main Industrial Use	Use in closed systems Chemical industry Intermediate
Remarks:	Intermediates in the manufacture of polyalphaolefins and other additives for lubricants, detergent alcohols, amine oxides and amines; C_{12} and C_{13} may be blended with other chemicals for use as drilling fluids for off-shore oil exploration.
(b) Main Industrial Use	Non-dispersive use Chemical industry – chemicals used in synthesis Intermediate
Remarks:	Intermediate in the manufacture of polyalphaolefins and other additives for lubricants, detergent alcohols, amine oxides and amines; C_{12} and C_{13} may be blended with other chemicals for use as drilling fluids for off-shore oil exploration.
Reference:	American Chemistry Council's Higher Olefins Panel (2002)

B. Uses In Consumer Products

Chemical not present in consumer products as marketed.

1.7 Sources of Exposure

Remarks: These products are produced commercially in closed systems and are used primarily as intermediates in the production of other chemicals. C_{12} and C_{13} olefins are blended with other chemicals for use as drilling fluids for off-shore oil exploration. No other non-intermediate applications have been identified. Any occupational exposures that do occur are most likely by the inhalation and dermal routes. It is a common practice to use personal protective equipment. In the case of dermal exposures, protective gloves would be worn due to the mildly irritating properties of this class of chemicals (ACC Higher Olefins Panel). Results from modelled data suggest that on-site waste treatment processes are expected to remove these substances from aqueous waste streams to the extent that they will not be readily detectable in effluent discharge (EPIWIN, 2000b). These substances are not on the US Toxic Release Inventory (TRI) list (NLM, 2003). These olefins will not persist in the environment because they can be rapidly degraded through biotic and abiotic processes.

Reference: American Chemistry Council's Higher Olefins Panel

1.8 Additional Information

A. Classification and Labelling

B. Occupational Exposure Limits

Exposure Limit Value

Type: None established
Value:

Short Term Exposure Limit Value

Value: None established

C. Options for Disposal

Remarks: Biotreater, burned for fuel

D. Last Literature Search

Type of search: Internal and external
Date of search: October 2003
Remark: Medline
IUCLID
TSCATS
ChemIDplus
AQUIRE - ECOTOX

E. Other Remarks

2. PHYSICAL CHEMICAL DATA

2.1 Melting Point

A. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Method: ASTM D97

GLP: Yes [ ] No[X]
Year: 1978

Results:

Melting point
Value: -50 °C:

Decomposition: Yes [ ] No [X] Ambiguous [ ]
Sublimation: Yes [ ] No [X] Ambiguous [ ]

Reliability: (4) Not assignable. These data were not reviewed for quality.

References: Enichem Augusta Industrials, Milan

B. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Method: ASTM D97

GLP: Yes [ ] No[X]
Year: 1978

Results:

Melting point
Value: -66 to -13°C:

Decomposition: Yes [ ] No [X] Ambiguous [ ]
Sublimation: Yes [ ] No [X] Ambiguous [ ]

Reliability: (2) Reliable with restrictions: Reliable source but these data were not reviewed for quality.

References: Shell Chemicals UK Ltd., Chester

C. Test Substance

Identity: CAS No. 28761-27-5, Undecene (mixture of isomers)

Method No data
GLP: No data
Year: No data

Results:

Melting point
Value: -77 °C

Decomposition: No data
Sublimation: No data

Reliability: (2) Reliable with restrictions. The result is experimental data as cited in the EPIWIN database. These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

References: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

D. Test Substance

Identity: CAS No. 25378-22-7, Dodecene or CAS No. 112-41-4, 1-Dodecene

Method

Method/
guideline followed: No data
GLP: No data
Year: No data

Test Conditions: No data

Results

Melting point
value in °C: -35.2°C [same value for both substances]

Reliability: (2) Reliable with restrictions: The result is measured data as cited in the EPIWIN database. These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

References: EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

E. Test Substance

Identity: CAS No. 25377-82-6, Tridecene

Method/
guideline followed: Calculated value using MPBPWIN version 1.41, a subroutine of the computer program EPIWIN version 3.11
GLP: Not applicable
Year: Not applicable

Test Conditions: Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb,

where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. Program used the structure for 1-tridecene.

Results

Melting point value in °C: -10.9°C

Reliability: (2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity: CAS No. 2437-56-1, 1-Tridecene

Method No data
GLP: No data
Year: No data

Results:

Melting point Value: -13 °C

Decomposition: No data
Sublimation: No data

Reliability: (2) Reliable with restrictions. The result is experimental data as cited in the EPIWIN database. These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

References: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity: CAS No. 68526-57-8; Alkenes, C10-12, C11-rich

Method/ guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of the computer program EPIWIN version 3.11
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. Program used the structure for 1-undecene.

Results

Melting point value in °C:	-33.69°C
Reliability:	(2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

H. Test Substance

Identity:	CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich
Method/ guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of the computer program EPIWIN version 3.11
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. Program used the structure for 1-dodecene.

Results

Melting point value in °C:	-22.16°C
Reliability:	(2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

I. Test Substance

Identity:	CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons
Method/ guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of the computer program EPIWIN version 3.11
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. Program used a C10 structure with double bonds in 5 locations.

Results

Melting point value in °C:	-48.73°C
Reliability:	(2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases

and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

J. Test Substance

Identity: CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

Method/ guideline followed: Calculated value using MPBPWIN version 1.41, a subroutine of the computer program EPIWIN version 3.11

GLP: Not applicable

Year: Not applicable

Test Conditions: Melting Point is calculated by the MPBPWIN subroutine, which is based on the average results of the methods of K. Joback, and Gold and Ogle, and chemical structure. Joback's Method is described in Joback, (1982). The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin. Program used a C12 structure with double bonds in 4 locations.

Results

Melting point value in °C: -24.15°C

Reliability: (2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.2 Boiling Point

A. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Method: ASTM D86

GLP: Yes [ ] No[X]
Year: 1982

Results:

Boiling point value: 183-236°C
Pressure Unit: 1013.25 hPa

Decomposition: Yes [ ] No [X] Ambiguous [ ]

Reliability: (4) Not assignable. These data were not reviewed for quality.

References: Enichem Augusta Industrials, Milan

B. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Method: ASTM D86

GLP: Yes [ ] No[X]
Year: 1982

Results:

Boiling point value: 170-233°C
Pressure Unit: 1013.25 hPa
Decomposition: Yes [ ] No [X] Ambiguous [ ]

Reliability: (2) Reliable with restrictions: Reliable source but these data were not reviewed for quality.

References: Shell Chemicals UK Ltd, Chester

C. Test Substance

Identity: CAS No. 28761-27-5, Undecene (mixture of isomers)
Method

Method: No data
GLP: No data
Year: No data

Results

Boiling point value: 194°C

Pressure:	1013
Pressure unit:	hPa
Reliability:	(2) Reliable with restrictions. The result is experimental data as cited in the EPIWIN database. These data were not reviewed for quality.
Flag:	Key study for SIDS endpoint.
References:	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

D. Test Substance

Identity:	CAS No. 25378-22-7, Dodecene or CAS No. 112-41-4, 1-Dodecene

Method

Method/ guideline followed:	No data
GLP:	No data
Year:	No data
Test Conditions:	No data

Results

Boiling point value in °C:	213.8°C [same value for both substances]
Pressure:	1013
Pressure unit:	hPa
Reliability:	(2) Reliable with restrictions. The result is measured data as cited in the EPIWIN database. These data were not reviewed for quality.
Flag:	Key study for SIDS endpoint
References:	EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

E. Test Substance

Identity:	CAS No. 25377-82-6, Tridecene

Method

Method/

guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11
GLP:	Not applicable
Year:	Not applicable

Test Conditions: Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used the structure for 1-tridecene.

Results

Boiling point value in °C:	224°C
Pressure:	1013
Pressure unit:	hPa

Reliability: (2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References:

Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity: CAS No. 2437-56-1, 1-Tridecene

Method

Method/ guideline followed:	No data
GLP:	No data
Year:	No data

Test Conditions: No data

Results

Boiling point value in °C:	233°C
Pressure:	1013
Pressure unit:	hPa

Reliability: (2) Reliable with restrictions. The result is measured data as cited in the EPIWIN database. These data were not reviewed for quality.

Flag:	Key study for SIDS endpoint
References:	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity:	CAS No. 68526-57-8; Alkenes, C10-12, C11-rich

Method

Method/ guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used the structure for 1-undecene.

Results

Boiling point value in °C:	184.07°C
Pressure:	1013
Pressure unit:	hPa
Reliability:	(2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.
	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

H. Test Substance

Identity:	CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich

Method

Method/ guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11
GLP:	Not applicable

Year:	Not applicable
Test Conditions:	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used the structure for 1-dodecene.
Results	
Boiling point value in °C:	204.24°C
Pressure:	1013
Pressure unit:	hPa
Reliability:	(2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587. EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

I. Test Substance

Identity:	CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons
Method	
Method/ guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used a C10 structure with double bonds in 5 locations.
Results	
Boiling point value in °C:	180.95°C
Pressure:	1013
Pressure unit:	hPa
Reliability:	(2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint

References: Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

J. Test Substance

Identity: CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

Method

Method/ guideline followed: Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11

GLP: Not applicable

Year: Not applicable

Test Conditions: Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of Stein and Brown (1994). Program used a C12 structure with double bonds in 4 locations.

Results

Boiling point value in °C: 229.23°C

Pressure: 1013

Pressure unit: hPa

Reliability: (2) Reliable with restrictions. The result is calculated data based on chemical structure as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Stein, S. and R. Brown (1994) Estimation of normal boiling points from group contributions (1994) J. Chem. Inf. Comput. Sci. 34: 581-587.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.3 Density (Relative Density)

A. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Method

Method:	ISO 3675
GLP:	Yes [ ] No [X] ? [ ]

Results

Type:	Bulk density [ ]; Density [x]; Relative Density [ ]
Value:	740 kg/m^3
Temperature:	20°C

Reliability: (4) Not assignable. These data were not reviewed for quality.

Reference: Shell Chemicals UK Ltd, Chester as cited in IUCLID

B. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Method

Method:	ISO 3675
GLP:	Yes [ ] No [X] ? [ ]

Results

Type:	Bulk density [ ]; Density [x]; Relative Density [ ]
Value:	750 kg/m^3
Temperature:	20°C

Reliability: (2) Reliable with restrictions: Reliable source but these data were not reviewed for quality.

Reference: Shell Chemicals UK Ltd, Chester

C. Test Substance

Identity: CAS No. 6842-15-5, Dodecene

Method

Method:	No data
GLP:	No data

Test Conditions: No data

Results

Type:	specific gravity
Value:	0.77
Temperature (°C):	20°C

Reliability: (2) Reliable with restrictions. Reliable secondary source. These data were not reviewed for quality.

Reference: U.S. Coast Guard Department of Transportation. CHRIS – Chemical Hazards Response Information System Washington, DC, information last updated 2002, website: http://www.chrismanual.com/default.htm.

D. Test Substance

Identity: CAS No. 112-41-4, 1-Dodecene

Method

Method: No data
GLP: No

Test Conditions: No data

Results
Type: density
Value: 0.76 g/cm^3
Temperature (°C): 20°C

Reliability: (2) Reliable with restrictions. Reliable secondary source. These data were not reviewed for quality.

Reference: Verschueren K (1983). Handbook of Environmental Data on Organic Chemicals, Van Nostrand Reinhold Company, Second Ed.

E. Test Substance

Identity: CAS No. 2437-56-1, 1-Tridecene

Method

Method: No data
GLP: No data

Results

Type: Bulk density [ ]; Density [ ]; Relative Density [x]
Value: 0.77
Temperature: 20°C

Reliability: (2) Reliable with restrictions: Reliable secondary source but these data were not reviewed for quality.

Reference: Lide, D.R. (ed.) (1998-1999) CRC Handbook of Chemistry and Physics. 79th ed. Boca Raton, FL: CRC Press Inc., p. 3-181.

F. Test Substance

Identity:	CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich

Method

Method:	No data
GLP:	No data

Results

Type:	Bulk density [ ]; Density [x]; Relative Density [ ]
Value:	0.77 g/cm^3
Temperature:	20°C
Reliability:	(2) Reliable with restrictions: Reliable source but these data were not reviewed for quality.
Reference:	ExxonMobil (2004) Dodecene Datasheet (unpublished data).

2.4 Vapour Pressure

A. Test Substance

Identity:	C10-13 n-olefins

Method

Method:	calculated by addition of the contributions (molar percentage) of the homologues
GLP:	Yes [ ] No [X]
Year:	1989

Results

Vapour Pressure value:	0.66 hPa
Temperature:	20^{o} C
Decomposition:	Yes [] *(temperature °C)* No [x] Ambiguous [ ]
Reliability:	(2) Reliable with restrictions: The value is calculated .
References:	Enichem Augusta Industrials, Milan

B. Test Substance

Identity:	CAS No. 28761-27-5, Undecene (mixture of isomers)

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN v. 3.11, MPBPWIN v 1.41
GLP:	Not applicable
Year:	Not applicable

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. The calculation used an experimental value for BP of 194 °C from EPIWIN database.

Results

Vapor Pressure value:	0.9172 hPa
Temperature (°C):	25°C
Remarks:	Reported as 0.688 mm Hg

Reliability: (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN using measured data as cited in the EPIWIN database. These data were not reviewed for quality.

Flag: Key study for SIDS endpoint

References:

Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

C. Test Substance

Identity: CAS No. 25378-22-7, Dodecene

Method

Method/ guideline followed:	Calculated value using MPBPWIN version 1.40, a subroutine of EPIWIN version 3.10
GLP:	Not applicable

Year:

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. The calculation used an experimental value for BP of 213.8 °C from the EPIWIN database.

Results

Vapor Pressure	
Value:	0.356 hPa
Temperature:	25°C
Remarks:	Reported as 0.267 mm Hg (25°C)

Reliability: (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References:

Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

D. Test Substance

Identity: CAS No. 112-41-4, 1-Dodecene

Method

Method/ guideline followed:	No data
GLP:	No data
Year:	No data

Test Conditions: No data

Results

Vapor Pressure	
Value:	0.212 hPa
Temperature:	25°C
Remarks:	Reported as 0.159 mm Hg (25°C)

Reliability: (2) Reliable with restrictions. The result is experimental data as cited in EPIWIN.

Flag: Key study for SIDS endpoint

References: Daubert, T.E. and R.P. Danner (1989) Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation; Design Institute for Physical Property Data, American Institute of Chemical Engineers. Hemisphere Pub. Corp., New York, NY; EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

E. Test Substance

Identity: CAS No. 25377-82-6, Tridecene

Method

Method/ guideline followed: Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11

GLP: Not applicable

Year:

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. The calculation used an experimental value for BP of 232.8 °C from the EPIWIN database.

Results

Vapor Pressure Value: 0.13999 hPa

Temperature: 25°C

Remarks: Reported as 0.105 mm Hg (25°C)

Reliability: (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References: Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity: CAS No. 2437-56-1, 1-Tridecene

Method

Method/ guideline followed: No data
GLP: No data
Year: No data

Test Conditions: No data

Results
Vapor Pressure
Value: 0.0851 hPa
Temperature: 25°C
Remarks: Reported as 0.0638 mm Hg (25°C)

Reliability: (2) Reliable with restrictions. The result is experimental data as cited in EPIWIN.

Flag: Key study for SIDS endpoint

References: Daubert, T.E. and R.P. Danner (1989) Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation; Design Institute for Physical Property Data, American Institute of Chemical Engineers. Hemisphere Pub. Corp., New York, NY; EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity: CAS No. 68526-57-8; Alkenes, C10-12, C11-rich

Method

Method/ guideline followed: Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11
GLP: Not applicable
Year:

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both

methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. The calculation used an experimental value for BP of 192.7 °C (for 1-undecene) from the EPIWIN database.

Results

Vapor Pressure	
Value:	0.9746 hPa
Temperature:	25°C
Remarks:	Reported as 0.731 mm Hg (25°C)

Reliability: (2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

Flag: Key study for SIDS endpoint

References:

Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

H. Test Substance

Identity: CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich

Method

Method/ guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11
GLP:	Not applicable
Year:	

Test Conditions: Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. The calculation used an experimental value for BP of 213.8 °C (for dodecene) from the EPIWIN database.

Results

Vapor Pressure	
Value:	0.356 hPa
Temperature:	25°C
Remarks:	Reported as 0.267 mm Hg (25°C)
Reliability:	(2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society. Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press. EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

I. Test Substance

Identity:	CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

Method

Method/ guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11
GLP:	Not applicable
Year:	
Test Conditions:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. The calculation used a value for BP of 180.95 °C estimated by EPIWIN using a C10 structure with double bonds in 5 locations.

Results

Vapor Pressure	
Value:	1.6932 hPa
Temperature:	25°C
Remarks:	Reported as 1.27 mm Hg (25°C)
Reliability:	(2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.

Flag:	Key study for SIDS endpoint
References:	Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society. Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press. EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

J. Test Substance

Identity:	CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

Method

Method/ guideline followed:	Calculated value using MPBPWIN version 1.41, a subroutine of EPIWIN version 3.11
GLP:	Not applicable
Year:	
Test Conditions:	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described by Lyman et al., 1990. A modified Grain Method is described by Neely and Blau, 1985. The calculation used a value for BP of 229.23 °C estimated by EPIWIN using a C12 structure with double bonds in 4 locations.

Results

Vapor Pressure Value:	0.1667 hPa
Temperature:	25°C
Remarks:	Reported as 0.125 mm Hg (25°C)
Reliability:	(2) Reliable with restrictions. The result is calculated data as modeled by EPIWIN.
Flag:	Key study for SIDS endpoint
References:	Lyman, W.J., W.F. Reehl and D.H. Rosenblatt, Eds. (1990) Handbook of Chemical Property Estimation. Chapter 14. Washington, D.C.: American Chemical Society.

Neely and Blau (1985) Environmental Exposure from Chemicals, Volume 1, p. 31, CRC Press.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.5 Partition Coefficient (log10Kow)

A. Test Substance

Identity:	CAS No. 28761-27-5, Undecene (mixture of isomers)

Method

Method:	Calculated value using the computer program EPIWIN version 3.11, KOWWIN v 1.67
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used the structure for 5-undecene.

Results

Log Kow:	5.53
Temperature (°C):	Not applicable
Reliability:	(2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.
Flag:	Key study for SIDS endpoint
Reference:	Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity:	CAS No. 25378-22-7, Dodecene or CAS No. 112-41-4, 1-Dodecene or CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich

Method

Method:	Calculated value using the computer program EPIWIN version 3.10, subroutine KOWWIN v 1.66
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). EPIWIN used structure for 1-dodecene.

Results

Log Kow:	6.10
Temperature (°C):	Not applicable
Reliability:	(2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.
Flag:	Key study for SIDS endpoint
Reference:	Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92. EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

C. Test Substance

Identity:	CAS No. 25377-82-6, Tridecene or CAS No. 2437-56-1, 1-Tridecene

Method

Method:	Calculated value using the computer program EPIWIN version 3.11, KOWWIN v 1.67
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used the structure for 1-tridecene.

Results

Log Kow:	6.59
Temperature (°C):	Not applicable

Reliability:	(2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.
Flag:	Key study for SIDS endpoint
Reference:	Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.
	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

D. Test Substance

Identity:	CAS No. 85535-87-1, Alkenes, C10-13
Method	
Method:	calculated fragment constants by Hansch and Leo
Year:	1979
Results	
Log Pow:	5.4 - 7
Temperature:	20 ^{o}C
Reliability:	(4) Not assignable. Results are calculated.
References:	Hansch C. and A. Leo (1979) *Substituent constants for correlation analysis in chemistry and biology*, Wiley, New York.
	Enichem Augusta Industrials, Milan, as cited in IUCLID

E. Test Substance

Identity:	CAS No. 68526-57-8; Alkenes, C10-12, C11-rich
Method	
Method:	Calculated value using the computer program EPIWIN version 3.11, KOWWIN v 1.67
GLP:	Not applicable
Year:	Not applicable

Test Conditions: Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used the structure for 1-undecene.

Results

Log Kow: 5.61
Temperature (°C): Not applicable

Reliability: (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.

Flag: Key study for SIDS endpoint

Reference: Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity: CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

Method

Method: Calculated value using the computer program EPIWIN version 3.11, KOWWIN v 1.67
GLP: Not applicable
Year: Not applicable

Test Conditions: Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used a C10 structure with double bonds in 5 locations.

Results

Log Kow: 4.33
Temperature (°C): Not applicable

Reliability: (2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.

Flag: Key study for SIDS endpoint

Reference:	Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.
	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity:	CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons
Method	
Method:	Calculated value using the computer program EPIWIN version 3.11, KOWWIN v 1.67
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of Meylan and Howard (1995). Program used a C12 structure with double bonds in 4 locations.
Results	
Log Kow:	5.37
Temperature (°C):	Not applicable
Reliability:	(2) Reliable with restrictions. The result was calculated based on chemical structure as modeled by EIPWIN.
Flag:	Key study for SIDS endpoint
Reference:	Meylan, W. and P. Howard (1995) Atom/fragment contribution method for estimating octanol-water partition coefficients. *J. Pharm. Sci.* 84:83-92.
	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.6.1 Water Solubility (including *Dissociation Constant).

A. Test Substance

Identity:	CAS No. 28761-27-5, Undecene (mixture of isomers)

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN 3.11, subroutine WSKOW v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 5.53 used for calculation. EPIWIN used structure for 5-undecene to calculate Log Kow.

Results

Value(mg/L) at temperature (°C):	0.4006 mg/L (25°C)
Reliability:	(2) Reliable with restrictions. The result is a calculated value.
Flag:	Key study for SIDS endpoint
References:	Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106. EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity:	CAS No. 25378-22-7, Dodecene

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN 3.11, subroutine WSKOW v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 6.10 used for

		calculation. EPIWIN used alpha structure to calculate Log Kow. Measured melting point of -35.2 °C used.
	Results	
	Value(mg/L) at temperature (°C):	0.1245 mg/L (25°C)
	Reliability:	(2) Reliable with restrictions. The result is a calculated value.
	Flag:	Key study for SIDS endpoint
	References:	Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106. EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.
C.	**Test Substance**	
	Identity:	2- Dodecene
	Method	
	Method/ guideline followed:	Calculated value using the computer program EPIWIN 3.10, subroutine WSKOW v 1.40
	GLP:	Not applicable
	Year:	Not applicable
	Test Conditions:	Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 6.02 used for calculation. Default values used for calculation
	Results	
	Value(mg/L) at temperature (°C):	0.1315 mg/L (25°C)
	Reliability:	(2) Reliable with restrictions. The result is a calculated value.
	References:	Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000a). Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

D. Test Substance

Identity: CAS No. 112-41-4, 1-Dodecene

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN 3.10, subroutine WSKOW v 1.40

GLP: Not applicable

Year: Not applicable

Test Conditions: Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 6.10 used for calculation. Default values used for calculation.

Results

Value(mg/L) at temperature (°C): 0.1127 mg/L (25°C)

Reliability: (2) Reliable with restrictions. The result is a calculated value.

Flag: Key study for SIDS endpoint

References:

Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000a). Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

E. Test Substance

Identity: CAS No. 25377-82-6, Tridecene or CAS No. 2437-56-1, 1-Tridecene

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN 3.11, subroutine WSKOW v 1.41

GLP: Not applicable

Year:	Not applicable
Test Conditions:	Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 6.59 used for calculation. EPIWIN used alpha structure to calculate Log Kow.
Results	
Value(mg/L) at temperature (°C):	0.03674 mg/L (25°C)
Reliability:	(2) Reliable with restrictions. The result is a calculated value.
Flag:	Key study for SIDS endpoint
References:	Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106. EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity:	CAS No. 68526-57-8; Alkenes, C10-12, C11-rich
Method	
Method/ guideline followed:	Calculated value using the computer program EPIWIN 3.11, subroutine WSKOW v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 5.61 used for calculation. EPIWIN used structure for 1-undecene to calculate Log Kow.
Results	
Value(mg/L) at temperature (°C):	0.3432 mg/L (25°C)
Reliability:	(2) Reliable with restrictions. The result is a calculated value.

Flag: Key study for SIDS endpoint

References: Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity: CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich

Method

Method/ guideline followed: Calculated value using the computer program EPIWIN 3.11, subroutine WSKOW v 1.41

GLP: Not applicable

Year: Not applicable

Test Conditions: Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 6.10 used for calculation. EPIWIN used structure for 1-dodecene to calculate Log Kow.

Results

Value(mg/L) at temperature (°C): 0.1127 mg/L (25°C)

Reliability: (2) Reliable with restrictions. The result is a calculated value.

Flag: Key study for SIDS endpoint

References: Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

H. Test Substance

Identity: CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN 3.11, subroutine WSKOW v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 4.33 used for calculation. EPIWIN used a C10 structure with double bonds in 5 locations. to calculate Log Kow.

Results

Value(mg/L) at temperature (°C):	5.2 mg/L (25°C)
Reliability:	(2) Reliable with restrictions. The result is a calculated value.
Flag:	Key study for SIDS endpoint
References:	Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106. EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

I. Test Substance

Identity:	CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

Method

Method/ guideline followed:	Calculated value using the computer program EPIWIN 3.11, subroutine WSKOW v 1.41
GLP:	Not applicable
Year:	Not applicable
Test Conditions:	Water Solubility is calculated by the WSKOW subroutine, which is based on a Kow correlation method described by Meylan et al., 1996. Estimated (EPIWIN) Log Kow value of 5.37 used for

calculation. EPIWIN used a C12 structure with double bonds in 4 locations to calculate Log Kow.

Results

Value(mg/L) at temperature (°C):	0.4989 mg/L (25°C)
Reliability:	(2) Reliable with restrictions. The result is a calculated value.
Flag:	Key study for SIDS endpoint
References:	Meylan, W., P. Howard and R. Boethling (1996) Improved method for estimating water solubility from octanol/water partition coefficient. *Environ. Toxicol. Chem.* 15:100-106.
	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

2.6.2 Surface tension

No data available

2.7 Flash Point (Liquids)

A. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Method

Method: ISO 2719
GLP: No data

Results

Value: 45°C
Type of test: Closed cup [X]; Open cup [ ]; Other [ ]

Reliability: (2) Reliable with restrictions: These data were not reviewed for quality.

Reference:

Remark: IUCLID cites Shell Chemicals UK Ltd, Chester

B. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Method

Method: ISO 2719
GLP: No data

Results

Value: 46°C
Type of test: Closed cup [X]; Open cup [ ]; Other [ ]

Reliability: (2) Reliable with restrictions: These data were not reviewed for quality.

Reference: Shell Chemicals UK Ltd, Chester

C. Test Substance

Identity: CAS No. 112-41-4, 1-Dodecene

Method

Method: ASTM D56
GLP:

Test Conditions: No data

Results

Value (°C): 77 °C
Type of test: Closed cup

Reliability: (2) Reliable with restrictions. Reliable secondary source. These data were not reviewed for quality.

Reference: Lappin, G.R. and J.D. Sauer (1989) Alpha Olefins Application Handbook, Marcel Dekker, Inc., N.Y.

D. Test Substance

Identity: CAS No. 2437-56-1, 1-Tridecene

Method

Method: No data
GLP: No data

Results

Value: ~175°C
Type of test: No data

Reliability: (2) Reliable with restrictions: Reliable secondary source. These data were not reviewed for quality.

Reference: U.S. Coast Guard Department of Transportation. CHRIS – Chemical Hazards Response Information System Washington, DC, information last updated 2002, website: http://www.chrismanual.com/default.htm.

2.8 Auto Flammability (Solids/Gases)

No data available

2.9 Flammability

No data available

2.10 Explosive Properties

No data available

2.11 Oxidising Properties

No data available

2.12 Oxidation-Reduction Potential

No data available

3. ENVIRONMENTAL FATE AND PATHWAYS

3.1 Stability

A. Photodegradation

(1) Test Substance

Identity: C11 – C13 alpha and internal olefins

Method

Method/
guideline followed: Other: Technical discussion

Type:	water
GLP:	Not applicable
Year:	Not applicable

Test Conditions: Not applicable

Results

Direct photolysis: In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Higher Olefins Category.

Remarks: The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (Harris, 1982a). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (Harris, 1982a). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (Harris, 1982a). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (Zepp and Cline, 1977).

Olefins with one double bond, such as the chemicals in the Higher Olefins category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerization about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (Harris, 1982a).

Products in the Higher Olefins Category do not contain component molecules that will undergo direct photolysis.

Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment.

Reliability: Not applicable

References: Harris J C (1982a). Rate of Aqueous Photolysis. Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA.

Zepp, R. G. and D. M. Cline (1977). Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.

(2) Test Substance

Identity: CAS No. 28761-27-5, Undecene (mixture of isomers)

Method

Method/
guideline followed: Calculated values using AOPWIN version 1.91, a subroutine of the computer program EIPWIN version 3.11 which uses a program described by Meylan and Howard (1993). Program used the structure for 5-undecene.

Type: air
GLP: Not applicable
Year: Not applicable

Results

Indirect photolysis

Sensitiser *(type):* OH
Rate Constant: 65.5690 E-12 cm^3/molecule-sec [Cis-isomer]
Degradation % after: 50% after 3.2 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm^3)
Rate Constant: 73.1690 E-12 cm^3/molecule-sec [Trans-isomer]
Degradation % after: 50% after 3.2 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm^3)

Sensitiser *(type):* Ozone
Rate Constant: 13 E-17 cm^3/molecule-sec [Cis-isomer]
Degradation % after: 50% after 2.116 hrs (using avg. OH conc. of 7 E11 mol/cm^3)

Rate Constant: 20 E-17 cm^3/molecule-sec [Trans-isomer]
Degradation % after: 50% after 1.375 hrs (using avg. OH conc. of 7 E11 mol/cm^3)

Reliability: (2) Reliable with restrictions. The value was calculated data based on chemical structure as modeled by EPIWIN. This robust summary has a rating of 2 because the data are calculated and not measured.

Flag: Critical study for SIDS endpoint

References: Meylan, W.M. and Howard, P.H. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 26: 2293-99

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

(3) Test Substance

Identity: CAS No. 25378-22-7, Dodecene or CAS No. 112-41-4, 1-Dodecene

Method

Method/
guideline followed: Calculated values using AOPWIN version 1.91, a subroutine of the computer program EIPWIN version 3.11 which uses a program described by Meylan and Howard (1993) . Program used the structure for 1-dodecene.

Type: air
GLP: Not applicable
Year: Not applicable

Results

Indirect photolysis

Sensitiser *(type):* OH
Rate Constant: 38.6563 E-12 cm^3/molecule-sec
. Degradation % after: 50% after 3.320 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm^3)

Sensitiser *(type):* Ozone
Rate Constant: 1.2 E-17 cm^3/molecule-sec
. Degradation % after: 50% after 22.920 hrs (using avg. ozone conc. of 7 E11 mol/cm^3)

Reliability: (2) Reliable with restrictions. The value was calculated data based on chemical structure as modeled by EPIWIN. This robust summary has a rating of 2 because the data are calculated and not measured.

Flag: Critical study for SIDS endpoint

References: Meylan, W.M. and Howard, P.H. (1993) Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 26: 2293-99

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

(4) Test Substance

Identity: CAS No. 25377-82-6, Tridecene or CAS No. 2437-56-1, 1-Tridecene

Method

Method/
guideline followed: Calculated values using AOPWIN version 1.91, a subroutine of the computer program EIPWIN version 3.11 which uses a program described by Meylan and Howard (1993). Program used the structure for 1-tridecene.

Type: air
GLP: Not applicable
Year: Not applicable

Results

Indirect photolysis

Sensitiser *(type):* OH
Rate Constant: 40.0693 E-12 cm^3/molecule-sec
Degradation % after: 50% after 3.2 hrs (using 12-hr day and avg. OH conc. of 1.5 E6 OH/cm^3)

Sensitiser *(type):* Ozone
Rate Constant: 1.2 E-17 cm^3/molecule-sec
Degradation % after: 50% after 22.92 hrs (using avg. OH conc. of 7 E11 mol/cm^3)35.8302

Reliability: (2) Reliable with restrictions. The value was calculated data based on chemical structure as modeled by EPIWIN. This robust summary has a rating of 2 because the data are calculated and not measured.

Flag: Critical study for SIDS endpoint

References:

Meylan, W.M. and Howard, P.H. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. Chemosphere 26: 2293-99

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Stability in Water

Test Substance

Identity: C11-C13 alpha or internal olefins

Method

Method/ guideline followed: Other – Technical Discussion
Type *(test type):*
GLP: Yes [ ] No[ ]
Year:

Test Conditions: Not applicable

Results: Not applicable

Remarks: Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (Gould, 1959; Harris, 1982b). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond. The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (Harris, 1982b) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Higher Olefins Category, will react with water by an addition reaction mechanism (Gould, 1959). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (Harris, 1982b). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates,

carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (Neely, 1985).

The substances in the Higher Olefins Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Higher Olefins Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

Conclusions: In the environment, hydrolysis will not contribute to the degradation of C11-C13 alpha or internal olefins.

Reliability: Not applicable

References:

Gould, E.S. (1959) Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA.

Harris, J.C. (1982b) "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA.

Neely, W. B. (1985) Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.

C. Stability In Soil

Data not available

3.2 Monitoring Data (Environment)

Data not available

3.3 Transport and Distribution

3.3.1 Transport between environmental compartments

A. Test Substance

Identity: CAS No. 28761-27-5, Undecene (mixture of isomers)

Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000b)

Chemical assumptions:

Molecular weight:	154.3
Water solubility:	0.401 g/m^3
Vapor pressure:	91.7Pa (25°C)
Log Kow:	5.53
Melting point:	-77°C

Half-life in air = 1.37 hr, half-life in water = 208 hr, half-life in soil = 208 hr, half-life in sediment = 832 hr
Environment name: EQC Standard Environment

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	95.9%	<1%
Water	<1%	26.7%
Soil	4.04%	46.8%
Sediment	<1%	26.1%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: These results indicated that undecene will partition primarily to air under equilibrium conditions (Level I model), but approximately half to soil and the remainder equally to water and sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References:

Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: CAS No. 25378-22-7, Dodecene

Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000b)

Chemical assumptions:

Molecular weight: 168
Water solubility: 0.125 g/m^3
Vapor pressure: 35.6 Pa (25°C)
Log Kow: 6.1
Melting point: -35.2°C
Environment name: EQC Standard Environment

Half-life in air = 5.149 hr, half-life in water = 360 hr, half-life in soil = 360 hr, half-life in sediment = 1440 hr

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	89%	<1%
Water	<1%	13%
Soil	10.3%	33.9%
Sediment	<1%	52.5%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: These results indicated that dodecene will partition primarily to air under equilibrium conditions (Level I model), but primarily to soil and sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia

Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

C. Test Substance

Identity: CAS No. 112-41-4, 1-Dodecene

Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000b)

Chemical assumptions:

Molecular weight: 168
Water solubility: 0.113 g/m^3
Vapor pressure: 21.2 Pa (25°C)
Log Kow: 6.1
Melting point: -35.2°C
Environment name: EQC Standard Environment

Half-life in air = 5.149 hr, half-life in water = 360 hr, half-life in soil = 360 hr, half-life in sediment = 1440 hr

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	Level III
Air	84.8%	<1%
Water	<1%	12.9%
Soil	14.9%	34.5%
Sediment	<1%	52.0%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: These results indicated that 1-dodecene will partition primarily to air under equilibrium conditions (Level I model), but primarily to soil and sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

D. Test Substance

Identity: CAS No. 25377-82-6, Tridecene

Method

Type: Fugacity models, Mackay Levels I and III

Remarks: Trent University model used for calculations. Half-lives in water, soil and sediment estimated using EPIWIN (EPIWIN, 2000b)

Chemical assumptions:

Molecular weight:	182
Water solubility:	0.0367 g/m^3
Vapor pressure:	14 Pa (25°C)
Log Kow:	6.59
Melting point:	-10.9°C

Half-life in air = 5.01 hr, half-life in water = 360 hr, half-life in soil = 360 hr, half-life in sediment = 1440 hr
Environment name: EQC Standard Environment

All other parameters were default values. Emissions for Level I = 1000 kg. Level III model assumed continuous 1000 kg/hr releases to each compartment (air, water and soil).

Results Media: Air, soil, water and sediment concentrations were estimated

	Level I	**Level III**
Air	79.9%	<1%
Water	<1%	9.8%
Soil	19.6%	26.8%
Sediment	<1%	63%

Remarks: Since default assumptions for release estimates were used, resulting environmental concentrations are not provided.

Conclusions: These results indicated that tridecene will partition primarily to air under equilibrium conditions (Level I model), but primarily to soil and sediment under the assumed pattern of chemical release (equal loading of water, soil and air) in the Level III model.

Reliability: (2) Valid with restrictions: Data are calculated.

Flag: Critical study for SIDS endpoint

References: Trent University (2004). Level I Fugacity-based Environmental Equilibrium Partitioning Model (Version 3.00) and Level III Fugacity-based Multimedia Environmental Model (Version 2.80.1. Environmental Modeling Centre, Trent University, Peterborough, Ontario. (Available at http://www.trentu.ca/cemc)

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

E. Test Substance

Identity: CAS No. 28761-27-5, Undecene (mixture of isomers)

Method

Type: Volatilization from water

Remarks: Calculated using the computer program EPIWIN version 3.11; based on Henry's Law Constant of 1.75 atm-m^3/mole (estimated by Bond SAR Method by EPIWIN).

Results: Half-life from a model river: 1.3 hrs
Half-life from a model lake: 4.9 days

Reliability: (2) Valid with restrictions: Values are calculated

References: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity: CAS No. 25378-22-7, Dodecene

Method

Type: Volatilization from water

	Remarks:	Calculated using the computer program EPIWIN version 3.10, using a Henry's Law Constant of 1.96 atm-m^3/mole (estimated by Bond SAR method).
	Results:	Half-life from a model river: 1.325 hrs Half-life from a model lake: 5.1 days
	Reliability:	(2) Valid with restrictions. Values are calculated.
	References:	EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10 Syracuse Research Corporation, Syracuse, NY. USA.

G. Test Substance

Identity:	CAS No. 25377-82-6, Tridecene
Method	
Type:	Volatilization from water
Remarks:	Calculated using the computer program EPIWIN version 3.11; based on Henry's Law Constant of 2.61 atm-m^3/mole (estimated by Bond SAR Method by EPIWIN).
Results:	Half-life from a model river: 1.4 hrs Half-life from a model lake: 5.3 days
Reliability:	(2) Valid with restrictions: Values are calculated
References:	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

3.3.2 Distribution

A. Test Substance

Identity:	CAS No. 28761-27-5, Undecene (mixture of isomers)
Method	
Method:	Adsorption Coefficient (Koc) calculated value using the computer program EPIWIN, PCKOC v 1.66 using the method described by Meylan et al., 1992.
Test Conditions:	Based on chemical structure. Program used the structure for 5-undecene.

Results

Value: Estimated Koc = 3179

Reliability: (2) Reliable with restrictions: Value is calculated.

Reference: Meylan, W., P.H. Howard and R.S. Boethling (1992) Molecular topology/fragment contribution method for predicting soil sorption coefficients. Environ. Sci. Technol. 26:1560-7.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: CAS No. 25378-22-7, Dodecene

Method

Method: Adsorption Coefficient (Koc) calculated value using the computer program EPIWIN, PCKOC v 1.66, based on the method of Meylan et al., 1992.

Test Conditions: Based on chemical structure. Program used the structure for 1-dodecene

Results

Value: Estimated Koc = 5864

Reliability: (2) Reliable with restrictions. Value is calculated.

Reference: Meylan, W., P.H. Howard and R.S. Boethling (1992) Molecular topology/fragment contribution method for predicting soil sorption coefficients. Environ. Sci. Technol. 26:1560-7

EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

C. Test Substance

Identity: CAS No. 25377-82-6, Tridecene

Method

Method: Adsorption Coefficient (Koc) calculated value using the computer program EPIWIN, PCKOC v 1.66 using the method described by Meylan et al., 1992.

Test Conditions: Based on chemical structure. Program used the structure for 1-tridecene.

Results

Value: Estimated Koc = 10,800

Reliability: (2) Reliable with restrictions: Value is calculated.

Reference: Meylan, W., P.H. Howard and R.S. Boethling (1992) Molecular topology/fragment contribution method for predicting soil sorption coefficients. Environ. Sci. Technol. 26:1560-7.

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

D. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Method: calculated Koc (soil partition coefficient)

Type: adsorption
Media: water-soil
Conditions: Brigg's Correlation : log Koc = 0.52 log Kow + 0.88 assuming log Kow = 7

Results

Value: Koc = 33,175

Reliability: (2) Reliable with restrictions: Result was calculated.

References: ENICHEM, Environmental partitioning model: a computer program prepared by Garlanda T and Mascero Garlanda M. (1990).

Remarks: IUCLID cites Shell Chemicals UK Ltd, Chester

E. Test Substance

Identity: CAS No. 85535-87-1, Alkenes, C10-13

Type: volatility
Media: water – air
Method: Calculated

Results

Value: Henry's Law constant = 11178 x 100 Pa x mc/mol

Reliability: (2) Reliable with restrictions: Result was calculated.

References: ENICHEM, Environmental partitioning model: a computer program prepared by Garlanda T and Mascero Garlanda M. (1990)

Remarks: IUCLID cites Enichem Augusta Industrials, Milan

F. Test Substance

Identity: CAS No. 28761-27-5, Undecene (mixture of isomers)

Method

Method: Henry's Law Constant calculated value using the computer program EPIWIN, HENRY v 3.11

Test Conditions: Bond and Group estimates based on chemical structure, at 25°C; VP/water solubility estimates based on values of VP = 0.688 mm Hg and WS = 0.401 mg/L. Program used the structure for 5-undecene.

Results

Value: Bond estimate = 1.75 atm-m^3/mole
Group estimate = 2.50 atm-m^3/mole
VP/Wsol estimate = 0.3487 atm-m^3/mole

Reliability: (2) Reliable with restrictions: Values are calculated.

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

G. Test Substance

Identity: CAS No. 25378-22-7, Dodecene

Method

Method: Henry's Law Constant calculated value using the computer program EPIWIN, HENRYWIN v 3.10

Test Conditions: Bond and Group estimates based on chemical structure, at 25°C; VP/water solubility estimates based on EPIWIN values of VP = 0.267 mm Hg and WS = 0.125 mg/L. Program used the structure for 1-dodecene.

Results

	Value:	Bond estimate = 1.96 atm-m^3/mole Group estimate = 4.25 atm-m^3/mole VP/Wsol estimate = 0. 475 atm-m^3/mole
	Reliability:	(2) Reliable with restrictions. Values are calculated.
	Reference:	EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

H. Test Substance

Identity:	CAS No. 25377-82-6, Tridecene
Method	
Method:	Henry's Law Constant calculated value using the computer program EPIWIN, HENRY v 3.11
Test Conditions:	Bond and Group estimates based on chemical structure, at 25°C; VP/water solubility estimates based on values of VP = 0.105 mm Hg and WS = 0.3067 mg/L. Program used the structure for 1-tridecene.
Results	
Value:	Bond estimate = 2.61 atm-m^3/mole Group estimate = 6.00 atm-m^3/mole VP/Wsol estimate = 0.686 atm-m^3/mole
Reliability:	(2) Reliable with restrictions: Values are calculated.
Reference:	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

3.4 Aerobic Biodegradation

A. Test Substance: C10-13 Internal Olefins (Shop Olefins 103 PQ11), linear

Remarks:	Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)
Method/guideline:	EEC Directive 84/449/EEC; Similar to OECD (301 D) Closed Bottle Test.
Test Type:	aerobic
GLP:	Yes
Year:	1984
Contact time:	28 days
Innoculum:	activated sludge

Test Conditions: Microorganisms were obtained from Sittingbourne Sewage Works (UK) and prepared according to standard test protocols. C10-13 Alpha Olefin was added to the test medium from a stock solution containing 2.4 g/L emulsified in Dobane PT sulphonate. The final test concentration was 2 mg olefins 103/L. Test bottles were incubated at 21±1°C and the extent of biodegradation was determined by measuring oxygen concentration in the bottles at days 5, 15 and 28. Controls with no microbial innoculum (control) and with medium plus microbial innoculum only (blank) were included. Sodium benzoate was used as a biodegradable substance to demonstrate the activity of the microbial innoculum.

Results: Under these test conditions, 103 PQ11Olefin was oxidized to 40% of the theoretical oxygen demand by day 5 and 65-70% by day 28 with no lag period. There was no significant inhibition of microbial activity under the test conditions. The report indicated that 103 Olefin was considered readily biodegradable; however, insufficient information was available to determine whether the 10-day window criterion was satisfied.

Reliability: (2) Reliable with restrictions: No information on kinetic of biodegradation or biodegradation of reference substance.

References: Miller RC, Watkinson RJ. (1984). Olefins 103 PQ 11: An Assessment of Ready Biodegradability. Shell Research Limited, Sittingbourne Research Center (unpublished report).

B. Test Substance

Identity: C10-13 Internal Olefins (Shop Olefins 103), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method/guideline: OECD 301D Closed Bottle Test
Type: Aerobic [X] Anaerobic [ ]
GLP: Yes
Year: 1985
Contact time: 28 days
Inoculum: Activated domestic sludge

Test Conditions: Microorganisms were obtained from Sittingbourne Sewage Works (UK) and prepared according to standard test protocols. C10-13 Olefin was added to the test medium from a stock solution containing 2.4 g/L emulsified in Dobane PT sulphonate. The final test concentration was 2 mg olefins 103/L. Test bottles were incubated at 21±1°C and the extent of biodegradation was determined by measuring oxygen concentration in the bottles at days 5, 15 and 28. Controls with no microbial innoculum

(control) and with medium plus microbial innoculum only (blank) were included. Sodium benzoate was used as a biodegradable substance to demonstrate the activity of the microbial innoculum.

Results: Under these test conditions, 103 Olefin was oxidized to 54% of the theoretical oxygen demand by day 5 and 60-67% by day 28 with no lag period. 89% of the possible oxygen demand had been consumed in the bottles titrated on day 15. Based on the 15-day results, the 10-day window criterion for "readily biodegradable" appears to have been met; however, the lower values found on day 28 confound the evaluation.

Reliability: (2) Reliable with restrictions: No information on kinetic of biodegradation or biodegradation of reference substance.

Reference: Turner, S.J., Watkinson, R.J., (1985) Shop Olefins 103: An assessment of Ready Biodegradability, Sittingbourne, Shell Research Limited, SBGR.85.106 (unpublished report).

C. Test Substance

Identity: CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich

Method

Method/guideline: OECD 301F, Ready Biodegradability, Manometric Respirometry Test
Type: Aerobic [X] Anaerobic [ ]
GLP: Yes
Year: 1993
Contact time: 28 days
Inoculum: Domestic activated sludge

Test Conditions: Activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, and calcium chloride).

Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.

Test material was tested in triplicate, controls and blanks were tested in duplicate.

Test material loading was approximately 50 mg/L. [Reason for using 50 mg/L instead of 100 mg/L: Substances such as this test material typically have ThODs between 2 and 3 mg per mg substance. Thus, the test material concentration was adjusted for a target of 100 mg THOD/L] Sodium benzoate (positive control) concentration was approximately 50 mg/L.

Test temperature was 22 +/- 1 Deg C.
All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results: Approximately 23% biodegradation of the test material was measured on day 28. By day 14, >60% biodegradation of the positive control was measured, which meets the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	19.0, 23.8, 25.3	22.7
Na Benzoate	91.0, 81.3	86.3

*replicate data

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

Reference: Exxon Biomedical Sciences, Inc. (1997) Ready Biodegradability: OECD 301F Manometric Respirometry. Study #115894A. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

D. Test Substance

Identity: CAS No. 68526-58-9; Alkenes, C12-14, C13 Rich

Method

Method/guideline: OECD 301F, Ready Biodegradability, Manometric Respirometry Test
Type: Aerobic [X] Anaerobic [ ]
GLP: Yes
Year: 1995
Contact time: 28 days
Inoculum: Domestic activated sludge

Test Conditions: Activated sludge and test medium were combined prior to test material addition. Test medium consisted of glass distilled water and mineral salts (phosphate buffer, ferric chloride, magnesium sulfate, and calcium chloride). Test vessels were 1L glass flasks placed in a waterbath and electronically monitored for oxygen consumption.Test material was tested in triplicate, controls and blanks were tested in duplicate. Test material loading was 45 mg/L. [Reason for using 45 mg/L instead of 100 mg/L: Substances such as this test material typically have ThODs between 2 and 3 mg per mg substance. Thus, the test material concentration was adjusted for a target of 100 mg THOD/L] Sodium

benzoate (positive control) concentration was approximately 50 mg/L. Test temperature was 22 +/- 1 Deg C. All test vessels were stirred constantly for 28 days using magnetic stir bars and plates.

Results: Approximately 8% biodegradation of the test material was measured on day 28.

Remarks: By day 14, >60% biodegradation of the positive control was measured, which meets the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
Test Material	6.28, 8.26, 8.35	7.63
Na Benzoate	88.2, 86.5	87.4

*replicate data

Reliability: (1) Reliable without restrictions

Reference: Exxon Biomedical Sciences, Inc. (1997) Ready Biodegradability: OECD 301F Manometric Respirometry. Study #119394A. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

E. Test Substance

Identity: CAS No. 28761-27-5, Undecene (mixture of isomers)
CAS No. 25378-22-7, Dodecene
CAS No. 112-41-4, 1-Dodecene
CAS No. 2437-56-1, 1-Tridecene
CAS No. 68526-57-8; Alkenes, C10-12, C11-rich
CAS No. 68526-58-9; Alkenes, C11-13, C12-rich

Method

Method/guideline: Estimated using the computer program EPIWIN v 3.11, BIOWIN v 4.01
Type: Aerobic

Test Conditions: Estimates use methods described by Howard et al., 1992; Boethling et al., 1994; and Tunkel et al., 2000. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.

Results: Linear model prediction: Biodegrades fast
Non-linear model prediction: Biodegrades fast
Ultimate biodegradation timeframe: Weeks
Primary biodegradation timeframe: Days
MITI linear model prediction: Biodegrades fast

MITI non-linear model prediction: Biodegrades fast

Reliability: (2) Reliable with restriction: Results are estimated

Flag: Key study for SIDS endpoint

Reference: Boethling, R.S., P.H. Howard, W. Meylan, W. Stiteler, J. Beaumann and N. Tirado (1994) Group contribution method for predicting probability and rate of aerobic biodegradation. Environ. Sci. Technol. 28:459-65.

Howard, P.H., R.S. Boethling, W.M. Stiteler, W.M. Meylan, A.E. Hueber, J.A. Beauman and M.E. Larosche (1992) Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data. Environ. Toxicol. Chem. 11:593-603.

Tunkel, J. P.H. Howard, R.S. Boethling, W. Stiteler and H. Loonen (2000) Predicting ready biodegradability in the MITI Test. Environ. Toxicol. Chem. (accepted for publication)

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

F. Test Substance

Identity: CAS No. 68514-32-9; C10,12 Olefin rich hydrocarbons
CAS No. 68514-33-0; C12,14 Olefin rich hydrocarbons

Method

Method/guideline: Estimated using the computer program EPIWIN v 3.11, BIOWIN v 4.01
Type: Aerobic

Test Conditions: Estimates use methods described by Howard et al., 1992; Boethling et al., 1994; and Tunkel et al., 2000. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.

Results: Linear model prediction: Biodegrades fast
Non-linear model prediction: Biodegrades fast
Ultimate biodegradation timeframe: Weeks (C10-12) or Days-Weeks (C12-14)
Primary biodegradation timeframe: Days-weeks
MITI linear model prediction: Does not biodegrade fast
MITI non-linear model prediction: Does not biodegrade fast

Reliability: (2) Reliable with restriction: Results are estimated

Flag: Key study for SIDS endpoint

Reference: Boethling, R.S., P.H. Howard, W. Meylan, W. Stiteler, J. Beaumann and N. Tirado (1994) Group contribution method for predicting probability and rate of aerobic biodegradation. Environ. Sci. Technol. 28:459-65.

Howard, P.H., R.S. Boethling, W.M. Stiteler, W.M. Meylan, A.E. Hueber, J.A. Beauman and M.E. Larosche (1992) Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data. Environ. Toxicol. Chem. 11:593-603.

Tunkel, J. P.H. Howard, R.S. Boethling, W. Stiteler and H. Loonen (2000) Predicting ready biodegradability in the MITI Test. Environ. Toxicol. Chem. (accepted for publication)

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

3.5 BOD5, COD or ratio BOD5/COD

No data available

3.6 Bioaccumulation

A. Test Substance

Identity: CAS No. 28761-27-5, Undecene (mixture of isomers)

Method

Method: BCF calculated value using the computer program EPIWIN, BCF v 2.15

Test Conditions: Based on chemical structure and a Log Kow of 5.53 estimated by EPIWIN, using methods described by Meylan et al., 1999. Formula used to make BCF estimate: Log BCF = 0.77 log Kow – 0.70 + correction (alkyl chains [8+ -CH2- groups] with a value of -1).

Results

Value: Estimated Log BCF = 2.557 (BCF = 360.5)

Reliability: (2) Reliable with restrictions: Results are calculated.

Reference: Meylan,WM, Howard,PH, Boethling,RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: CAS No. 25378-22-7, Dodecene

Method

Method: BCF calculated value using the computer program EPIWIN, BCF v 2.15

Test Conditions: Based on chemical structure and a Log Kow of 6.1 (estimated by EPIWIN program using structure for 1-dodecene) using methods described by Meylan et al., 1999. Formula used to make BCF estimate: Log BCF = 0.77 log Kow – 0.70 + correction (alkyl chains [8+ -CH2- groups] with a value of -1.5).

Results

Value: Estimated Log BCF = 2.496 (BCF = 313.1)

Reliability: (2) Reliable with restrictions. Value is calculated.

Reference: Meylan,WM, Howard,PH, Boethling,RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

C. Test Substance

Identity: CAS No. 25377-82-6, Tridecene

Method

Method: BCF calculated value using the computer program EPIWIN, BCF v 2.15

Test Conditions: Based on chemical structure and a Log Kow of 6.59 estimated by EPIWIN, using the structure for 1-tridecene and methods described by Meylan et al., 1999. Formula used to make BCF estimate: Log BCF = 0.77 log Kow – 0.70 + correction (alkyl chains [8+ -CH2- groups] with a value of -1.5).

Results

Value: Estimated Log BCF = 2.874 (BCF = 747.8)

Reliability: (2) Reliable with restrictions: Results are calculated.

Reference: Meylan,WM, Howard,PH, Boethling,RS et al. (1999) Improved method for estimating bioconcentration / bioaccumulation factor from octanol/water partition coefficient. Environ. Toxicol. Chem. 18(4): 664-672

EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

3.7 Additional Information

A. Sewage Treatment

Test Substance

Identity: CAS No. 28761-27-5, Undecene (mixture of isomers)

Test Method: Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility. Input values: MW = 154.3; Henry's LC = 1.75 atm-m^3/mol; air-water partition coefficient = 71.5698; Log Kow =5.53; biomass to water partition coefficient = 67769.7; temperature = 25°C

GLP: No

Test Medium: Secondary waste water treatment (water)

Test Type: Aerobic

Test Results: 99.87 % removed from wastewater treatment

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Test Substance

Identity: CAS No. 25378-22-7, Dodecene

Test Method: Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility.

Input values: MW = 168.33; Henry's LC = 1.96 atm-m^3/mol; air-water partition coefficient = 80.158; Log Kow = 6.1; biomass to water partition coefficient = 251,786; temperature = 25°C

GLP: No

Test Medium: Secondary waste water treatment (water)

Test Type: Aerobic

Test Results: 99.74 % removed from wastewater treatment

Reference: EPIWIN (2000a) Estimation Program Interface for Windows, version 3.10. Syracuse Research Corporation, Syracuse, NY. USA.

C. Sewage Treatment

Test Substance

Identity: CAS No. 25377-82-6, Tridecene

Test Method: Calculated, EPIWIN STP Fugacity Model, predicted fate in a wastewater treatment facility. Input values: MW = 182.35; Henry's LC = 2.61 atm-m^3/mol; air-water partition coefficient = 106.741; Log Kow =6.59; biomass to water partition coefficient = 778,091; temperature = 25°C

GLP: No

Test Medium: Secondary waste water treatment (water)

Test Type: Aerobic

Test Results: 99.51 % removed from wastewater treatment

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

4. ENVIRONMENTAL TOXICITY

4.1 Acute Toxicity to Fish

A. Test Substance

Identity: Olefins 103 PQ 11 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated

Type (test type): Semi-static Fish Acute Toxicity Test

GLP: Not stated

Year (study performed): 1984

Species: Rainbow Trout (*Salmo gairdneri*)

Analytical Monitoring: No

Exposure Period: 96 Hours

Statistical Method: Visual inspection

Test Conditions: Control and dilution water was laboratory mains tap water obtained from bore holes in the chalk of North Downs (U.K.). Water was dechlorinated and passed through particle and activated carbon filters (alkalinity 253 mg/L as $CaCO_3$, hardness 274 mg/L as $CaCO_3$, conductivity 510 µS/cm, pH 7.3). Test vessels were glass aquaria each filled with 10 L of water and contained 10 fish per vessel. Quantities of test substance were added directly to six aquaria to give concentrations of 20, 50, 100, 200, 500, and 1000 mg/L. The seventh aquarium served as a control and received no test substance. The fish were not fed during the test. Test fish had a mean length of 3.0 cm (range 2.5 to 3.3 cm) and a mean weight of 0.23 g (range 0.15 to 0.32 g). Fingerlings were obtained from Itchen Valley Trout Farm, Alresford, Hampshire, U.K. and acclimated to test conditions for more than 10 days before use. One replicate per treatment and control was used. The aquaria were gently aerated to maintain dissolved oxygen concentration. At 24 h intervals, the number of dead fish was recorded and any dead removed, dissolved oxygen and pH were measured in the old and fresh solutions of the control and high concentration, and the test solutions were renewed. Temperature in one test aquarium was monitored at 4h intervals throughout the test. Total hardness was determined in each batch of fresh media. Test temperature was 13-17 Deg C. Dissolved oxygen ranged from 10.0 to 10.4 mg/L in the fresh media and 9.8 to 10.2 mg/L in the old solutions. pH was 8.2 – 8.4. Total hardness was 240-260 mg/L as $CaCO_3$. Photoperiod was not stated in the test report.

Results:

Units/Value: 96h LC50 was > solubility; LL0 = 1000 mg/L

Remarks: Observations made during the study suggest the test substance was not wholly soluble at concentrations of approximately 20 mg/L and greater as indicated by an oily film visible on the surface of the test solutions. Concentrations were expressed as the amount of test substance added. No fish died during the 96h exposure in the 1000 mg/L treatment. The 96h LC50 was > solubility. There were also 100% survival in the control, 50, 100, 200 and 500 mg/L treatments. One fish died (10% mortality) in the 20 mg/L treatment. Although the report did not state whether the study was conducted under GLP, a quality assurance statement was included stating that study procedures were inspected and the report was audited.

Reliability: (2) Reliable with restrictions. Test substance was not wholly soluble at the concentrations tested. A more appropriate and currently accepted method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Other shortcomings of the study include: 1) only one replicate per concentration was used, and 2) analytical verification of the test substance in the exposure solutions was not performed.

Reference: Shell Research Limited (1984) Olefins 103 PQ 11: Acute toxicity to *Salmo gairdneri, Daphnia magna* and *Selenastrum capricornutum.* Sittingbourne Research Centre, SBGR.83.359 (unpublished report).

Other: This study was included in the dossier for 1-decene at SIAM 11. Additional information has been added.

B. Test Substance

Identity: SHOP Olefins 103 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated
Type (test type): Semi-static Fish Acute Toxicity Test
GLP: Not stated
Year (study performed): 1985
Species: Rainbow Trout (*Salmo gairdneri*)
Analytical Monitoring: No
Exposure Period: 96 Hours
Statistical Method: Visual inspection

Test Conditions: Control and dilution water was laboratory mains tap water obtained from bore holes in the chalk of North Downs (U.K.). Water was dechlorinated and passed through particle and activated carbon filters (alkalinity 255 mg/L as $CaCO_3$, hardness 270 mg/L as $CaCO_3$, conductivity 545 µS/cm, pH 7.4). Test vessels were glass aquaria each filled with 10 L of water and contained 10 fish per vessel. Quantities of test substance were added directly to two aquaria to give concentrations of 500 and 1000 mg/L. A third aquarium served as a control and received no test substance. The fish were not fed during the test. Test fish had a mean length of 4.1 cm (range 3.9 to 4.5 cm) and a mean weight of 0.66 g (range 0.47 to 0.86 g). Fingerlings were obtained from Itchen Valley Trout Farm, Alresford, Hampshire, U.K. and acclimated to test conditions for more than 10 days before use. One replicate per treatment and control was used. The aquaria were gently aerated to maintain dissolved oxygen concentration. At 24 h intervals, the number of dead fish was recorded and any dead removed, dissolved oxygen and pH were measured in the old and fresh solutions of the control and high concentration, and the test solutions were renewed. Temperature in one test aquarium was monitored at 4h intervals throughout the test. Total hardness was determined in each batch of fresh media. Test temperature was 18.5±1.0 Deg C. Dissolved oxygen ranged from 9.6 to 10.2 mg/L in the fresh media and 9.0 to 9.8

mg/L in the old solutions. pH was 7.4 – 8.4. Total hardness was 222-262 mg/L as $CaCO_3$. Photoperiod was not stated in the test report.

Results:

Units/Value: 96h LC50 was > solubility; LL0 = 1000 mg/L

Remarks: The test substance was not wholly soluble at the test concentrations and was visible as floating droplets. Concentrations were expressed as the amount of test substance added. Only one fish died during the 96h exposure in the 1000 mg/L treatment. The 96h LC50 was > solubility. There was 100% survival in the control and 500 mg/L treatment.

Reliability: (2) Reliable with restrictions. Test substance was not wholly soluble at the concentrations tested. A more appropriate and currently accepted method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Other shortcomings of the study include: 1) only two concentrations were tested, 2) only one replicate per concentration was used, and 3) analytical verification of the test substance in the exposure solutions was not performed.

Reference: Shell Research Limited (1985) SHOP Olefins 103: Acute toxicity (*Salmo gairdneri, Daphnia magna* and *Selenastrum capricornutum*) and n-octanol/water partition coefficient. Sittingbourne Research Centre, SBGR.85.182 (unpublished report).

Other: This study was included in the dossier for 1-decene at SIAM 11. Additional information has been added.

C. Test Substance

Identity: CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich

Method

Method/guideline: OECD 203
Test type: Semi-static Fish Acute Toxicity Test
GLP: Yes [X] No [ ]
Year: 1995
Species/Strain: *Oncorhynchus mykiss* (Rainbow trout)
Analytical Monitoring: Yes
Exposure period: 96 hours
Statistical methods: No mortality occurred; therefore, statistical analysis of the data was not warranted.

Test Conditions: This test was conducted as a limit test, i.e., one test material exposure solution was tested. The test solution was prepared by adding the test

substance, via syringe, to 19.5 L of laboratory blend water in a 20 L glass carboy. The solution was mixed for 24 hours with a vortex of ≤10%. Mixing was performed using a magnetic stir plate and Teflon® coated stir bar at room temperature (approximately 22C). After mixing, the solution was allowed to settle for one hour after which the Water Accommodated Fraction (WAF) was siphoned from the bottom of the mixing vessel through a siphon that was placed in the carboy prior to adding the test material. Test vessels were 4.0 L aspirator bottles that contained approximately 4.5 L of test solution. Each vessel was sealed with no headspace after 5 fish were added. Three replicates of the test material loading were prepared. Approximately 80% of each solution was renewed daily from a freshly prepared WAF.

The test material loading level was 86.0 mg/L. A control containing no test material was included. The analytical results were below the lowest quantitation standard (0.20 mg/L).

Test temperature was 16C. Lighting was 666 to 669 Lux with a 16-hr light and 8-hr dark cycle. Dissolved oxygen ranged from 9.0 to 9.8 mg/L for "new" solutions and 6.1 to 7.4 mg/L for "old" solutions. The pH ranged from 7.6 to 8.3 for "new" solutions and 7.3 to 7.9 for "old" solutions.

Fish supplied by Thomas Fish Co., Anderson, CA, USA; age at test initiation = approximately 5 weeks; mean wt. at test termination = 0.271 g; mean total length at test termination = 3.1 cm; test loading = 0.32 g of fish/L. The fish were slightly shorter than the guideline suggestion of 4.0 to 6.0 cm, which were purposely selected to help maintain oxygen levels in the closed system. Fish size had no significant effect on study outcome.

Results:

96-hour LL0 = 86.0 mg/L based upon loading rates; LC50 > solubility.

Analytical method used was Headspace Gas Chromatography with Flame Ionization Detection (GC-FID).

Loading Rate (mg/L)	Measured Conc. (mg/L)	Fish Total Mortality (@96 hrs)*
Control	ND	0
86.0	BD	0

* 15 fish added at test initiation
ND - not detected; the lowest analyzed standard was 0.20 mg/L
BD - below the lowest analyzed standard, 0.20 mg/L

Remarks:

The test material is not sufficiently water soluble to cause mortality to rainbow trout in a 96-hour acute toxicity test. Although the water solubility of this test material at a loading of 86.0 mg/L was not established, the sum of its components at this loading is likely to be less

than 0.20 mg/L because this was the lowest standard used in the analyses that supported this study.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Exxon Biomedical Sciences, Inc. (1996) Fish, Acute Toxicity Test. Study #119258. Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA (unpublished report).

4.2 Acute Toxicity to Aquatic Invertebrates (e.g. Daphnia)

A. Test Substance

Identity: Olefins 103 PQ 11 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated
Type (test type): Static Daphnid Acute Toxicity Test
GLP: Not stated
Year (study performed): 1983
Species: Water Flea (*Daphnia magna*)
Analytical Monitoring: No
Exposure Period: 48 hours
Statistical Method: Probit analysis

Test Conditions: Nominal loading rates in the definitive test were 0, 0.05, 0.1, 0.2, 0.5, 1, 2, and 5 mg/L. Control and dilution water was reconstituted hard water prepared by adding salts to glass-distilled deionized water following EPA guidelines (hardness 170 mg/L as $CaCO_3$). Quantities of stock solutions of the test substance in acetone were added to triplicate sets of 140 ml conical flasks and made up to 140ml with dilution water. Three flasks served as controls and received no test substance. Acetone concentration in control and test flasks was 0.1 ml/L. Ten daphnids, less than 24h old, were placed in each flask. Daphnids were obtained from laboratory cultures and collected from cultures aged between 15 and 35 days. Young for testing were not taken from cultures containing adults with ephippia. In order to minimize daphnids from potentially being trapped in undissolved test substance at the surface of the test solutions, loosely fitting black paper caps were placed over the flasks to create a darkened zone which the daphnids would avoid. After 24 and 48h, the numbers of immobilized daphnids were recorded. Temperature in one test vessel was monitored at 4h intervals. The pH and dissolved oxygen concentration in a control and highest treatment were determined at test

initiation and termination. Total hardness of the dilution water used was measured at the beginning of the test. Test temperature was 18 – 22 Deg C. Photoperiod was 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 8.8 to 9.2 mg/L. pH was 8.0 – 8.3. Total hardness of the water was 170 mg/L as $CaCO_3$.

Results:

Units/Value: 48-h EL50 = 0.74 mg/L (nominal)

Remarks: No undissolved test substance was observed even at 5 mg/L, the highest concentration tested.. Concentrations were expressed as the amount of test substance added. 48-h EL50 = 0.74 mg/L (nominal) with 95% confidence limits of 0.61-0.88 mg/L. There was no immobilization of *D. magna* in the control, 0.05, and 0.1mg/L after 48-h. There were 1 (3.3%), 7 (23.3%), 19 (63.3%), 30 (100%) and 30 (100%) daphnids immobilized in the 0.2, 0.5, 1, 2, and 5 mg/L, respectively. Although the report did not state whether the study was conducted under GLP, a quality assurance statement was included stating that study procedures were inspected and the report was audited.

Reliability: (2) Reliable with restrictions. This study was well documented and comparable to a guideline study. Information provided indicate that test concentrations did not appear to have exceeded water solubility of the test substance as evidenced by absence of undissolved material in the exposure solutions. However, analytical verification of the test substance in the test solutions was not performed.

Flag: Key study for SIDS endpoint

Reference: Shell Research Limited (1984) Olefins 103 PQ 11: Acute toxicity to *Salmo gairdneri, Daphnia magna* and *Selenastrum capricornutum.* Sittingbourne Research Centre, SBGR.83.359 (unpublished report).

Other: This study was included in the dossier for 1-decene at SIAM 11. Additional information has been added.

B. Test Substance

Identity: SHOP Olefins 103 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated
Type (test type): Static Daphnid Acute Toxicity Test
GLP: Yes

Year (study performed): 1985
Species: Water Flea (*Daphnia magna*)
Analytical Monitoring: No
Exposure Period: 48 hours
Statistical Method: Probit analysis

Test Conditions: Nominal loading rates in the definitive test were 0, 1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460 and 1000 mg/L. Control and dilution water was reconstituted hard water prepared by adding salts to glass-distilled deionized water following EPA guidelines (hardness 168-169 mg/L as $CaCO_3$). Before use, a soil extract was added to the reconstituted fresh water at 20 ml/L. The soil extract was prepared by autoclaving 100 g soil/L distilled water for 15 min at 120 deg C and filtered through Whatman GF/C filter. Quantities of stock solutions of the test substance in Analar acetone were added to triplicate sets of 140 ml glass flasks and made up to 140ml with dilution water. Three flasks served as controls and received no test substance. Acetone concentration in control and test flasks was 0.1 ml/L. Ten daphnids, less than 24h old, were placed in each flask. Daphnids were obtained from laboratory cultures and collected from cultures aged between 15 and 35 days. Young for testing were not taken from cultures containing adults with ephippia. In order to minimize daphnids being trapped in the surface layer of test substance visible at all test concentrations, loosely fitting black caps were placed over the flasks to create a darkened zone which the daphnids would avoid. After 24 and 48h, the numbers of immobilized daphnids were recorded. Temperature in one test vessel was monitored at 4h intervals. The pH and dissolved oxygen concentration in a control and highest treatment were determined at test initiation and termination. Total hardness of the dilution water used was measured at the beginning of the test. Test temperature was 18 – 22 Deg C. Photoperiod was 16 hrs light and 8 hrs dark. Dissolved oxygen ranged from 8.6 to 9.0 mg/L. pH was 8.0 – 8.4. Total hardness of the water was 170 mg/L as $CaCO_3$.

Results:

Units/Value: 48-h EL50 = 480 mg/L (nominal)

Remarks: The test substance was not wholly soluble at all test concentrations and was visible at the surface. Concentrations were expressed as the amount of test substance added. 48-h EL50 = 480 mg/L with 95% confidence limits of 400-580 mg/L. There was no immobilization of *D. magna* in the control, 1.0, 2.2, 4.6, 10, 22, 46 and 100 mg/L after 48-h. There were 3 (10%), 14 (46.7%), and 27 (90%) daphnids immobilized in the 220, 460, and 1000 mg/L, respectively.

Reliability: (3) Not Reliable. Test substance was not wholly soluble at the concentrations tested despite the use of a solvent carrier to prepare stock solutions. A more appropriate and currently accepted method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Analytical

verification of the test substance in the exposure solutions was also not performed.

Reference: Shell Research Limited (1985) SHOP Olefins 103: Acute toxicity (*Salmo gairdneri, Daphnia magna* and *Selenastrum capricornutum*) and n-octanol/water partition coefficent. Sittingbourne Research Centre, SBGR.85.182 (unpublished report).

Other: This study was included in the dossier for 1-decene at SIAM 11. Additional information has been added.

4.3 Toxicity to Aquatic Plants (e.g. Algae)

A. Test Substance

Identity: Olefins 103 PQ 11 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated
Type (test type): Algal Toxicity Test
GLP: Not stated
Year (study performed): 1983
Species: Freshwater Green Alga (*Selenastrum capricornutum*)
Analytical Monitoring: No
Exposure Period: 4 days
Statistical Method: EL50 values determined by probit analysis

Test Conditions: Control and dilution water was algal nutrient medium prepared by dissolving Analar grade salts in glass-distilled deionized water according to EPA guidelines except that boric acid was present at 105 µg/L and sodium bicarbonate at 50 mg/L. Sixteen Erlenmeyer flasks containing 50 ml of culture medium were prepared. Quantities of stock solutions of the test substance in acetone were added to ten flasks to give concentrations of 1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460, and 1000 mg/L. Six flasks served as controls and received no test substance. Acetone concentration in the control and treatment flasks was 0.1 ml/L. Each flask was inoculated with algal cells to yield an initial concentration of 500 cells/ml. Algal cells were obtained from laboratory cultures that were originally derived from a strain from American Type Culture Collection (ATCC 22662). Flasks were incubated in a cooled orbital (100 cycles/min) incubator under constant illumination (~3000 lux) at 22-26 deg C (monitored at 4h intervals). After 2 and 4 days incubation, cell counts were made using a Coulter Counter. The initial pH in the control and highest concentration was 7.9 – 8.0. The 96h EC50 (concentration

causing a 50% reduction in cell number at day 4 compared to mean control cell number at day 4) was calculated using log transformed concentration values.

Results:

Units/Value: 96h EL50 based on cell numbers at day 4 was 24 mg/L

Remarks: The test substance was not wholly soluble at concentrations of approximately 20 mg/L and greater as indicated by an oily film visible on the surface of the test solutions. Concentrations were expressed as the amount of test substance added. The 96h EC50 based on cell numbers at day 4 was 24 mg/L with 95% confidence limits of 2.9-79 mg/L).

Nominal Conc. (mg/L)	Day 4 Cell Conc. (cells/ml x 10^6)	Day 4 cell number as % Day 4 mean control cell number
Control	1.03(mean)	
1.0	1.1	112
2.2	1.1	110
4.6	1.1	108
10	0.87	85
22	0.33	32
46	0.092	9
100	0.13	13
220	0.11	11
460	0.093	9
1000	0.096	9

Although the report did not state whether the study was conducted under GLP, a quality assurance statement was included stating that study procedures were inspected and the report was audited.

Reliability: (3) Not Reliable. Test substance was not wholly soluble at some of the concentrations tested despite the use of a solvent carrier to prepare stock solutions. A more appropriate and currently accepted method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Other shortcomings of the study include: 1) only one replicate per concentration was used, and 2) analytical verification of the test substance in the exposure solutions was not performed.

Reference: Shell Research Limited (1984) Olefins 103 PQ 11: Acute toxicity to *Salmo gairdneri, Daphnia magna* and *Selenastrum capricornutum.* Sittingbourne Research Centre, SBGR.83.359 (unpublished report).

B. Test Substance

Identity: SHOP Olefins 103 (C10-C13 linear internal olefins)

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method/Guideline: Not stated

Year (guideline): Not stated
Type (test type): Algal Toxicity Test
GLP: Yes
Year (study performed): 1985
Species: Freshwater Green Alga (*Selenastrum capricornutum*)
Analytical Monitoring: No
Exposure Period: 4 days
Statistical Method: EC50 values determined by probit analysis

Test Conditions: Control and dilution water was algal nutrient medium prepared by dissolving Analar grade salts in glass-distilled deionized water according to EPA guidelines except that boric acid was present at 105 µg/L and sodium bicarbonate at 50 mg/L. Sixteen Erlenmeyer flasks containing 50 ml of culture medium were prepared. Quantities of stock solutions of the test substance in Analar acetone were added to ten flasks to give concentrations of 1.0, 2.2, 4.6, 10, 22, 46, 100, 220, 460, and 1000 mg/L. Six flasks served as controls and received no test substance. Acetone concentration in the control and treatment flasks was 0.1 ml/L. Each flask was inoculated with algal cells to yield an initial concentration of 500 cells/ml. Algal cells were obtained from laboratory cultures that were originally derived from a strain from American Type Culture Collection (ATCC 22662). Flasks were incubated in a cooled orbital (100 cycles/min) incubator under constant illumination (~3000 lux) at 22.0-26.5 deg C (monitored at 4h intervals). After 2 and 4 days incubation, cell counts were made using a Coulter Counter. The pH in the control and highest concentration ranged from 7.4 – 7.6 at test initiation and 7.1 – 7.4 at test termination. The 96h EC50 (concentration causing a 50% reduction in cell number at day 4 compared to mean control cell number at day 4) was calculated using log transformed concentration values.

Results:

Units/Value: 96h EL50 based on cell numbers at day 4 was 22 mg/L

Remarks: The test substance was not wholly soluble at 220, 460, and 1000 mg/L and was visible as floating droplets which precluded cell counting. Concentrations were expressed as the amount of test substance added. The 96h EC50 based on cell numbers at day 4 was 22 mg/L with 95% confidence limits of 19-24 mg/L).

Nominal Conc. (mg/L)	Day 4 Cell Conc. (cells/ml x 10^6)	Day 4 cell number as % Day 4 mean control cell number
Control	1.25(mean)	
1.0	1.4	115

2.2	1.1	92
4.6	1.4	111
10	1.1	87
22	0.63	51
46	0.12	10
100	0.015	1

Reliability: (3) Not Reliable. Test substance was not wholly soluble at some of the concentrations tested despite the use of a solvent carrier to prepare stock solutions. A more appropriate and currently accepted method for preparing test solutions for multi-component test substances with low water solubility is the use of water accommodated fractions. Other shortcomings of the study include: 1) only one replicate per concentration was used, and 2) analytical verification of the test substance in the exposure solutions was not performed.

Reference: Shell Research Limited (1985) SHOP Olefins 103: Acute toxicity (*Salmo gairdneri, Daphnia magna* and *Selenastrum capricornutum*) and n-octanol/water partition coefficent. Sittingbourne Research Centre, SBGR.85.182 (unpublished report).

Other: This study was included in the dossier for 1-decene at SIAM 11. Additional information has been added.

C. Test Substance

Identity: CAS No. 112-41-4, 1-Dodecene (>97%, Neraten®12)

Method

Method/guideline: No data
Test type: static
GLP: No
Year: 1997
Analytical Monitoring: No data
Species/Strain: Planktonic freshwater green algae, *Scenedesmus subspicatus,* from collection

of autotrophic organisms of the Botanical Institute of AV ČR.
Element basis: 10,000 cells per 1mL, area under the curve, exponential growth rate
Exposure period: 72hrs
Statistical methods: Inhibition of algae growth in % was calculated as integral of biomass (area under growth curve) I_{ai}. The terminal inhibition evaluation was done by software Toxicita VÚV Ostrava (1991). For calculation of E_bC50, used approximation function: multinominal 3.stage with a 95% confidence limit.

Test Conditions: Algae inoculum was taken from an exponentially growing culture, after a 3-day pre-cultivation. Cell density was measured immediately before the start of the test and the necessary volume of inoculum, corresponding to

10,000 cells per 1mL, was determined. Every concentration set had control tests without tested material. Sensitivity of algae culture and accuracy of the test execution was checked by testing of standard material (potassium dichromate p.a.).

Test temperature range: 21-25°C, pH of solutions: 7.70.

Un-watered standard nutrient medium for algae cultivation, prepared by mixing of reserve solutions A, B, C, D in volume 100,10,10,10 and complementing to 1L with distilled water:

Reserve solution A:		Reserve solution B:	
NH_4Cl	1.5g	$FeCl_3 .6H_20$	80mg
$MgCl_2.6H_20$	1.2g	$Na_2EDTA.2H_20$	100mg
$CaCl_2.2H_20$	1.8g	in 1L distilled water	
K_2HPO_4 0.16g			
in 1L distilled water			

Reserve solution C:		Reserve solution D:	
H_3BO_3	185mg	NaHCO3	50g
$MnCl_2$	415mg	in 1L distilled water	
$ZnCl_2$	3mg		
$CoCl_2.6H_20$	1.5mg		
$CuCl_2.2H_20$	0.01mg		
$Na_2Mo0_4.2H_20$	7mg		
in 1L distilled water			

Dilution water was obtained by dilution of un-watered nutrient solution with water (1:10).

Equipment: Agitator LT-2, pH meter WTW-pH 539, fluor tube of universal white light of range 6000-10000 lux, microscope, Burker's computing chamber, equipment for microfiltration, filters Synpor with pores 0.2um, bulbs, beakers, pipettes.

Duration of the test is 72hrs. The sample was taken and the density of algae suspension was determined microscopically as number of cells in 1mL every 24hrs.

Results:

E_bL50 (0-72hrs)=15.4 mg/l (confidence limits: 14. 25-16.58)
E_rL50 (0-72hrs) could not be determined

Remarks:

Base solution 0.0183g/l diluting water.
Preliminary test:

Thinning	ml/l	1000	500	100	Control	
Concentration		mg/l	18.3	9.15	1.8	
Number of cells		0hr	10000	10000	10000	10000
Number of cells		72hrs	125000	156250	181250	193750

Base test I:

Thinning ml/l	1000	800	600	400	200	100	Control
Concentration mg/l	18.3	14.6	10.9	7.3	3.7	1.8	0
Number of cells/ml (0hr)	10000	10000	10000	10000	10000	10000	10000
Number of cells/ml (72hrs)	18750	137500	143750	162500	181250	187500	206250

Inhibition I_{ai} %	69.3	42.6	35.6	26.7	13.8	10.9	0
Inhibition I_{ui} %	18.8	13.9	11.9	7.9	3.9	2.9	0
Base test II:							
Thinning ml/l	1000	800	600	400	200	100	Control
Concentration mg/l	18.3	14.6	10.9	7.3	3.7	1.8	0
Number of cells/ml (0hr)	10000	10000	10000	10000	10000	10000	10000
Number of cells/ml (72hrs)	125000	131250	143750	168750	175000	175000	200000
Inhibition I_{ai} %	69.4	43.9	33.7	23.5	12.2	12.2	0
Inhibition I_{ui} %	16	14	11	6	5	5	0

Reliability: (3) Not reliable. Because this study cites an effect that was seen above the water solubility limit, the results are questionable.

References: Research Institute of Organic Synthesis a.s (1997) Pardubice, Czech Republic test Protocol No. 28/L (unpublished report).

4.4 Toxicity to Micro-organisms, e.g. Bacteria

Test Substance

Identity: CAS No. 85535-87-1, Alkenes C10-13, linear internal olefins

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method: Inhibition of growth
GLP: No data
Species: *Pseudomonas fluorescens*
Exposure Period: No data
Analytical Monitoring: No data

Results: Maximum inhibition was 19% at 1000 mg/L

Reliability: (4) Not assignable

Reference: Turner, S.J., Watkinson, R.J., (1985) Shop Olefins 103: An assessment of Ready Biodegradability, Sittingbourne, Shell Research Limited, SBGR.85.106 (unpublished report).

Other: This study was included in the dossier for 1-decene at SIAM 11.

4.5 Chronic Toxicity to Aquatic Organisms

A. Chronic Toxicity to Fish

(1) **Test Substance:** CAS No. 28761-27-5, Undecene (mixture of isomers) ; or CAS No. 68526-57-8; Alkenes, C10-12, C11-Rich

Method/Guideline:

Type (test type): 30-day Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: Fish

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used Kow values of 5.53 for undecene and 5.61 for Alkenes, C10-12, C11 Rich. The Kow values were estimated by EPIWIN using the structure for 5-undecene for undecene, and the structure for 1-undecene for the C11-Rich substance.

Results:

Units/Value: Estimated 30-day ChV for undecene = 13 µg/L
Estimated 30-day ChV for Alkenes, C10-12, C11-Rich = 11 µg/L

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

(2) **Test Substance:** CAS No. 25378-22-7, Dodecene ; CAS No. 112-41-4, 1-Dodecene; or CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich

Method/Guideline:

Type (test type): 30-day Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: Fish

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used a Kow value of 6.10, which was estimated by EPIWIN using the structure for 1-dodecene.

Results:

Units/Value: Estimated 30-day ChV = 4 µg/L for all three substances

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

(3) **Test Substance:** CAS No. 25377-82-6, Tridecene ; or CAS No. 2437-56-1, 1-Tridecene

Method/Guideline:

Type (test type): 30-day Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: Fish

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used a Kow value of

6.59, which was estimated by EPIWIN using the structure for 1-tridecene.

Results:

Units/Value: Estimated 30-day ChV = 2 µg/L for both substances

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Chronic Toxicity to Aquatic Invertebrates

(1) **Test Substance:** CAS No. 28761-27-5, Undecene (mixture of isomers) ; or CAS No. 68526-57-8; Alkenes, C10-12, C11-Rich

Method/Guideline:

Type (test type): 16-day EC50 value calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: *Daphnia magna*

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used Kow values of 5.53 for undecene and 5.61 for Alkenes, C10-12, C11 Rich. The Kow values were estimated by EPIWIN using the structure for 5-undecene for undecene, and the structure for 1-undecene for the C11-Rich substance.

Results:

Units/Value: Estimated 16-day EC50 for undecene = 18 µg/L
Estimated 16-day EC50 for Alkenes, C10-12, C11-Rich = 16 µg/L

	Flag:	Key study for SIDS endpoint
	Reliability:	(2) Reliable with restrictions. The result is calculated data.
	Reference:	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.
(2)	**Test Substance:**	CAS No. 25378-22-7, Dodecene; CAS No. 112-41-4, 1-Dodecene; or CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich
	Method/Guideline:	
	Type (test type):	16-day EC50 value calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)
	Species:	*Daphnia magna*
	Test Conditions:	The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used a Kow value of 6.10, which was estimated by EPIWIN using the structure for 1-dodecene.
	Results:	
	Units/Value:	Estimated 16-day EC50 = 8 μg/L for all three substances
	Flag:	Key study for SIDS endpoint
	Reliability:	(2) Reliable with restrictions. The result is calculated data.
	Reference:	EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.
(3)	**Test Substance:**	CAS No. 25377-82-6, Tridecene ; or CAS No. 2437-56-1, 1-Tridecene

Method/Guideline:

Type (test type): 16-day EC50 value calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: *Daphnia magna*

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used a Kow value of 6.59, which was estimated by EPIWIN using the structure for 1-tridecene.

Results:

Units/Value: Estimated 16-day EC50 = 4 µg/L for both substances

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

4.6 Toxicity to Terrestrial Organisms

A. Toxicity to Terrestrial Plants.

(1) **Test Substance:** CAS No. 28761-27-5, Undecene (mixture of isomers) ; or CAS No. 68526-57-8; Alkenes, C10-12, C11-Rich

Method/Guideline:

Type (test type): 96-hr Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: Green algae

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used Kow values of 5.53 for undecene and 5.61 for Alkenes, C10-12, C11 Rich. The Kow values were estimated by EPIWIN using the structure for 5-undecene for undecene, and the structure for 1-undecene for the C11-Rich substance.

Results:

Units/Value: Estimated 96-hr ChV for undecene = 44 µg/L
Estimated 96-hr ChV for Alkenes, C10-12, C11-Rich = 39 µg/L

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

(2) **Test Substance:** CAS No. 25378-22-7, Dodecene; CAS No. 112-41-4, 1-Dodecene; or CAS No. 68526-58-9; Alkenes, C11-13, C12 Rich

Method/Guideline:

Type (test type): 96-hr Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: Green algae

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used a Kow value of

6.10, which was estimated by EPIWIN using the structure for 1-dodecene.

Results:

Units/Value: Estimated 96-hr ChV = 21 µg/L for all three substances

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

(3) **Test Substance:** CAS No. 25377-82-6, Tridecene ; or CAS No. 2437-56-1, 1-Tridecene

Method/Guideline:

Type (test type): 96-hr Chronic Toxicity Value (ChV) calculated using the computer program ECOSAR, version 0.99g included in the EPI Suite software, v 3.11 (EPIWIN, 2000b)

Species: Green algae

Test Conditions: The program uses structure-activity relationships (SARs) to predict the aquatic toxicity of chemicals based on their similarity of structure to chemicals for which the aquatic toxicity has been previously measured. The program uses regression equations developed for chemical classes using the measured aquatic toxicity values and estimated Kow values. Toxicity values for new chemicals are calculated by inserting the estimated Kow into the regression equation and correcting the resultant value for the molecular weight of the compound. The CAS number was used for input into EPIWIN. The program used a Kow value of 6.59, which was estimated by EPIWIN using the structure for 1-tridecene.

Results:

Units/Value: Estimated 96-hr ChV = 11 µg/L for both substances

Flag: Key study for SIDS endpoint

Reliability: (2) Reliable with restrictions. The result is calculated data.

Reference: EPIWIN (2000b). Estimation Program Interface for Windows, version 3.11. EPI Suite™ software, U.S. Environmental

Protection Agency, Office of Pollution Prevention and Toxics, U.S.A.

B. Toxicity to Soil Dwelling Organisms.

No data available

C. Toxicity to Other Non Mammalian Terrestrial Species (including Avian)

No data available

4.7 Biological Effects Monitoring (including Biomagnification)

No data available

4.8 Biotransformation and Kinetics

No data available

5. MAMMALIAN TOXICITY

5.1 Toxicokinetics, Metabolism and Distribution

No data available

5.2 Acute Toxicity

A. Acute oral toxicity

(1) Test Substance: C10-13 Internal Olefins (Shop Olefins 103 PQ11), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method/guideline:	NA
Type *(test type):*	LD50
GLP:	Pre-GLP
Year:	1977
Species/Strain:	Rat/Wistar
Sex:	Males and females
No. of animals per sex per dose:	4

Vehicle:	none
Route of administration:	Oral gavage
Test Conditions:	Male and female rats, aged approximately 12 weeks, were used at each dose level (5 and 10 ml/kg). The animals were weighed, fasted overnight and the calculated dose of material administered by intraesophagael intubation using a ball point needle fitted to a syringe. After dosing food and water were freely available throughout a 9 day observation period.
Results:	
Value:	LD50 > 7740 mg/kg
Number of deaths at each dose level:	1 at 10 ml/kg
Remarks:	Animals showed no signs of toxic reaction during the 9 day observation period. One female rat died following a period of not eating and drinking and loss of body weight. Under the conditions of this study, C10-13 Olefins have a low order of toxicity.
Reliability:	(1) Reliable without restrictions.
Flag:	Key study for SIDS endpoint
References:	Shell Toxicology Laboratory, Tunstall (1977) Toxicology of alpha olefins: Acute toxicity, skin and eye irritancy and skin sensitizing potential of alpha olefin 103 PQ 11 (unpublished report).
Other:	This study was included in the dossiers for 1-decene and 1-dodecene at SIAM 11. Additional information has been added.

(2) **Test Substance**

Identity (purity):	CAS No. 25377-82-6, Tridecene (100%), NEODENE® 13 Internal Olefin
Method	
Method/guideline:	TSCA Health Effects Test Guidelines, 40 CFR 798.1175, meeting OECD Guidelines, Section 401
Type *(test type):*	LD50
GLP:	Yes
Year:	1995
Species/Strain:	Albino Rat / Crl:CD®BR
Sex:	Males and females
No. of animals per	

sex per dose:	5
Vehicle:	NA
Route of administration:	Oral gastric intubation

Test Conditions: Single treatment dose level of 5000 mg/kg. Based on specific gravity of 0.75 g/ml, the dose volume was 6.67 ml/kg. Weight of young adult animals ranged from 248 to 295 grams at initiation of dosing.

Prior to dosage, food was withheld from the animals for approximately 18-20 hours. Four hours following exposure, food and water were made available. The animals were observed for gross effects and mortality at 1, 3, and 4 hours on study day 0 and once daily thereafter for 14 days. Body weights were obtained on study days –1, 0, 7, and 14. Upon termination, all rats were euthanized by carbon dioxide asphyxiation. The major organ systems of the cranial, thoracic and abdominal cavities were examined for all animals.

Results:

Value:	LD50 > 5000 mg/kg
Number of deaths at each dose level:	None

Remarks: All animals survived to the scheduled necropsy. All rats had yellow urogenital and/or ventral abdominal staining on days 0 and/or 1. Various hair loss on the urogenital, ventral abdominal and/or hindlimb (right and/or left) areas was noted for six animals. Three rats had dried red material around the nose. There were no other clinical findings. With the exception of hair loss noted on the hindlimb(s), urogenital and/or ventral abdominal areas from days 5 to 14, all animals appeared normal by day 2. There were no remarkable changes or differences observed in body weights. At study termination (day 14), the coagulating gland was absent in one male. This absence was considered a congenital abnormality. Various hair loss on the hindlimb(s) and/or ventral abdominal areas was observed on four rats at the scheduled necropsy. There were no other gross necropsy findings for all examined tissues.

Under the conditions of this study, tridecene has a low order of toxicity.

Reliability: (1) Reliable without restrictions, comparable to guideline study

Flag: Key study for SIDS endpoint

References: WIL Research Laboratories, Inc. (1995) Acute Oral Toxicity Study of NEODENE®13 Internal Olefin in Albino Rats; Performed for Shell Chemical Co. (unpublished report).

(3) **Test Substance**

Identity (purity): CAS No. 68526-58-9, Alkenes, C11-13, C12 rich

Method

Method/guideline:	NA
Type *(test type):*	LD50
GLP:	Pre-GLP
Year:	1961
Species/Strain:	Rat/Sprague-Dawley
Sex:	Males
No. of animals per sex per dose:	5
Vehicle:	Corn oil
Route of administration:	Oral gavage

Test Conditions: Age of the test animals was not reported. Body weights ranged from 103 to 126g at initiation of the study. Frequency of treatment: Single treatment. Dose/Concentration Levels:Either 0.1, 1.0, and 10.0% volume/volume in corn oil or undiluted. (Equivalent to 24.5, 77.4, 245, 774, 2446, and 7440 mg/kg). For the purpose of this study, the test material was considered to be free of impurities. Control group and Treatment: For comparison, untreated animals were necropsied at the end of the study. Prior to dosage, food was withheld from the animals for three hours. Following exposure, food and water was available at all times. The animals were observed for gross effects and mortality at 1, 4, and 24 hours and once daily thereafter for 7 days. Gross necropsies were performed at the end of the observation period. Tissue samples from the 2446 and 7440 mg/kg dose levels were collected for further analysis.

No mortality occurred; therefore, statistical analysis of the data was not warranted.

Results:

Value:	LD50 > 7740 mg/kg
Number of deaths at each dose level:	None

Remarks:	Animals at all dosage levels exhibited normal appearance and behavior throughout the entire study and showed normal body weight gain. There were no pathological findings at necropsy. Under the conditions of this study, Alkenes, C11-13, C12-rich have a low order of toxicity.
Reliability:	(1) Reliable without restrictions, comparable to guideline study
Flag:	Key study for SIDS endpoint
References:	Hazleton Laboratories, Inc. (1961) Acute Oral Administration - Rats, Acute Dermal Application - Rabbits, Acute Eye Application - Rabbits, Acute Inhalation Exposure - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co. (unpublished report).

(4) Test Substance

Identity (purity):	CAS No. 112-41-4, 1-Dodecene (C12 alpha olefin)

Method

Method/guideline:	OECD 401
Type *(test type):*	LD50
GLP:	No
Year:	1976
Species/Strain:	Sprague-Dawley Rat
Sex:	Male
No. of animals per sex per dose:	10
Vehicle:	None
Route of administration:	Oral gavage
Test Conditions:	Groups of 10 male Sprague Dawley rats weighing 200-300 g were gavaged, after overnight fasting, with 1-dodecene, neat, at 10 g/kg body-weight. The animals were observed for 14 days after dosing. Survivors were sacrificed and autopsied.
Results:	There were no deaths and no visible signs of toxicity. All of the animals were gaining weight normally. The autopsy did not reveal any gross pathological changes.
Value:	LD50 > 10 g/kg
Number of deaths at each dose level:	0/10

Reliability:	(2) Reliable with restrictions: Incomplete reporting of experimental details
Flag:	Key study for SIDS endpoint
References:	Carter, G. (1976) A report on the acute toxicity of Alpha Olefin C12, Ethyl Corporation (unpublished report).
Other:	This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

B. Acute inhalation toxicity

(1) **Test Substance:**	C10-13 Internal Olefins (Shop Olefins 103), linear
Remarks:	Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method/guideline:	4-hr exposures in a dynamic exposure system.
Type *(test type):*	LC50
GLP:	No
Year:	1980
Species/Strain:	Rat/Wistar
Sex:	Males and females
No. of animals per sex per dose:	5
Vehicle:	None
Route of administration:	Inhalation (mist)

Test Conditions: One group of 10 rats each (5 males and 5 females, approximately 10 weeks of age) was exposed for 4 hrs to a saturated concentration of test substance (> 2.1 mg/L, ~305 ppm). Animals were observed for 14 days post-exposure. Initial, 7 day and 14 day body weights were recorded.

The animals were contained within 7 liter glass chambers fitted with carriers to accommodate five animals each, through which the test atmosphere was passed at a minimal rate of 10 liters/minute.

The test atmosphere was generated by flash vaporization of the test substance supplied to a heated flask by means of a micro metering pump. The vapor was blended with dilution air in a mixing flask, and the vapor/air mixture was passed through an air cooled condenser and a condensation trap to the inhalation

chambers. Continuous analysis of the atmosphere during exposure was undertaken exposure using a heated total hydrocarbon analyzer.

Results:

Value:	LC50 >2.1 mg/L (~305 ppm) (saturated concentration) mist.
Number of deaths at each dose level:	None
Remarks:	Some rats lachrymated and salivated during exposure, but no other toxic signs were observed during the 14 day observation period.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Blair, D., Sedgewick, A.E. (1980) The acute inhalation toxicity of Olefins 103 PQ 11. Sittingbourne, Shell Research Limited, TLGR.80.052 (unpublished report).
Other:	This study was included in the dossier for 1-decene at SIAM 11. Additional information has been added.

(2) Test Substance

Identity (purity):	CAS No. 68526-58-9, Alkenes, C11-13, C12 rich

Method

Method/guideline:	NA
Type *(test type):*	LC50
GLP:	Pre-GLP
Year:	1961
Species/Strain:	Swiss Albino Mice, Wistar Rats, English short hair guinea pigs
Sex:	Males
No. of animals per sex per dose:	10/species
Vehicle:	NA
Route of administration:	Inhalation (saturated vapors only, no aerosol)
Test Conditions:	Age of the test animals was not reported. Mean body weights were 26g (mice), 154g (rats), and 327g (guinea pigs) at initiation of the study. Dose/Concentration Levels: 4.4 mg/L for 6 hours (saturated vapors only, no aerosol). Control group and Treatment: Control animals (5/sex/species) were exposed to clean air at the same flow rate as the treated group. Air was

bubbled through the test material and into a chamber to give a total flow through the chamber of 35 liters/minute. The theoretical mean chamber concentration (4.4 mg/L, 639 ppm) was calculated from the loss of material and airflow through the chamber. Animals were observed throughout the exposure period for signs of toxicity. Following the exposure period, animals were observed for signs of toxicity daily for 14 days. Gross necropsies were performed on any animals that died during the study and all animals at the completion of the study. For the purpose of this study, the test material was considered to be free of impurities.

No mortality occurred; therefore, statistical analysis of the data was not warranted.

Results:

Value: $LC_{50} > 4.4$ mg/L (639 ppm) for 6 hours

Number of deaths at each dose level: None

Remarks: Immediately following initiation of the exposure, all animals exhibited increased motor activity. Lacrimation was observed in rats and guinea pigs beginning at the 90-minute interval. Otherwise, all animals seemed normal in appearance and behavior throughout the study. No abnormalities were observed at necropsy. Under the conditions of this study, Alkenes, C11-13, C12 rich have a low order of acute inhalation toxicity in rats.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint.

References: Hazleton Laboratories, Inc. (1961) Acute Oral Administratio-- - Rats, Acute Dermal Applicatio-- - Rabbits, Acute Eye Applicatio-- - Rabbits, Acute Inhalation Exposur-- - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co. (unpublished report).

(3) Test Substance

Identity (purity): C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

Remarks: Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

Method

Method/guideline:	1-hr exposures to seven different concentrations in a dynamic exposure system.
Type *(test type):*	LC50
GLP:	Yes [ ] No [X]
Year:	1967
Species/Strain:	Rat/Wistar
Sex:	Males
No. of animals per sex per dose:	Not reported
Vehicle:	None
Route of administration:	Inhalation

Test Conditions: Groups of male albino Wistar rats weighing between 209 and 299 g were exposed for 1 hour to saturated mists of the test substance and observed for 14 days. The number of animals per group was not reported. The animals were observed for toxic signs during exposure and were periodically weighed for 14 days after exposure. On the ^{14}th day, they were sacrificed for the determination of gross pathological changes.

The saturated mists were prepared by placing a Dautrabanda nebulizer within the exposure chamber and passing an air line and olefin feed line to it from outside. This aerosol generator produces particles no larger than 8 μ in diameter. It was found experimentally that the maximum mist concentration was achieved when the nebulizer was operating at an air flow of 2 L/min with about 50 ml of olefin in the reservoir. Estimates of mist concentration were made from measurement of the volume loss from the nebulizer reservoir and total air flow through the system. Additionally, a sample holder containing a millipore filter was positioned downward in the chamber and air drawn through at a rate calculated to collect suspended particles of 2 μ or less. The lower size limit of collection by the filter was expected to be 0.45μ . Papers were weighed before and after collection and the weight gain used to calculate concentration of particles in the 0.45-2.0 μ range. Statistical methods were not used.

Results:

Value:	LC50 >9900 mg/m^3 (1438 ppm)
Number of deaths at each dose level:	None
Remarks:	The aerosol generator produced particles that were <8 microns in diameter. Rats showed a drowsy appearance on removal from the chamber. The drowsiness/ lethargy disappeared rapidly when

animals were removed from exposure. The fur of animals was "oily" from deposition of particles. There was no mortality and no significant weight change or gross pathological change on autopsy. Estimated exposure concentrations were 9900 mg/m^3 for particles <8μ and 100 mg/m^3 for particles 0.4– - 2.0μ . These concentrations represented very heavy mists. Visability through the chamber (12" diameter) was impossible. The LC50 was > 9900 mg/m^3.

Reliability: (2) Reliable with restrictions: No information is given on the number of animals dosed and there are limited details of procedures.

References: Rinehart, W.E. (1967) Toxicological Studies on Several Alpha Olefins. University of Pittsburgh, submitted to Gulf Research and Development Co. (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

C. Acute dermal toxicity

(1) Test Substance: C10-13 Internal Olefins (Shop Olefins 103 PQ 11), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method/guideline:	Noakes and Sanderson
Type (test type):	LD50
GLP:	Pre-GLP
Year:	1977
Species/Strain:	Rat/ Wistar
Sex:	Males and females
No. of animals per sex per dose:	4
Vehicle:	NA
Route of administration:	Dermal

Test Conditions: Groups of animals, aged 12-13 weeks, were exposed to the test substance in single exposures to concentrations of 1, 2, and 4 ml/kg. Undiluted test material was applied to shorn dorso-lumbar skin and bandaged into contact with the skin using an impermeable dressing of aluminum foil and water proof plaster. Following the 24-hour exposure period, the dressings were

removed and the exposed area was sponged with tepid dilute detergent solution to remove residue. Animals were observed for gross signs of s toxicity daily for 9 days.

Results:

Value:	LD_{50} > 3080 mg/kg
Number of deaths at each dose level:	4 mortalities occurred in the female rats at dose level 4 ml/kg; one each at day 6 and day 8, 2 at day 7.
Remarks:	Rats showed no signs of toxic reactions, but those that eventually died did not eat or drink and lost body weight. On the basis of these figures, the acute percutaneous LD50 was estimated to be greater than 4 ml/kg (3080 mg/kg) in males and between 2 and 4 ml/kg (between 1540 and 3080 mg/kg) in females.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Shell Toxicology Laboratory, Tunstall (1977) Toxicology of alpha olefins: Acute toxicity, skin and eye irritancy and skin sensitizing potential of alpha olefin 103 PQ 11 (unpublished report).

(2) Test Substance

Identity (purity):	CAS No. 25377-82-6, Tridecene (100%), NEODENE®13 Internal Olefin

Method

Method/guideline:	TSCA Health Effects Test Guidelines, 40 CFR 798.1111, meeting OECD Guidelines, Section 402
Type *(test type):*	LD50 and No Observable Effect Level (NOEL)
GLP:	Yes
Year:	1995
Species/Strain:	Albino Rat / Crl:CD®BR
Sex:	Males and females
No. of animals per sex per dose:	5
Vehicle:	NA
Route of administration:	Dermal
Test Conditions:	One group of young adult male and female albino rats was dermally administered single doses of test substance at a dose level of 2000 mg/kg. Based on a measured specific gravity of 0.75 g/ml, the dose volume was 2.67 ml/kg. Individual body weights were obtained just prior to dosing and on study days 0, 7

and 14 post-dosing. Weights ranged from 239 to 275 grams at initiation of dosing. Undiluted test material was applied to clipped, intact dorsal skin and covered approximately 20% of the total body surface. The test substance was held in contact with the skin under semi-occlusive dressing consisting of gauze bandaging that was secured with non-irritating tape. Collars were applied and remained on the rats for the duration of the exposure (24 hrs) to prevent ingestion of the test substance. Upon completion of the exposure period, the collars and bandages were removed and the application sites were wiped with disposable paper towels moistened with tepid water.

Animals were observed for mortality and systemic toxicity at approximately 1.0, 3.0, and 4.0 hours post-dose on study day 0 and twice daily (morning and afternoon) thereafter for14 days. The application sites were examined for erythema, edema and other dermal findings beginning approximately 30-60 minutes after bandage removal and daily thereafter for 13 days. The rats were clipped to facilitate dermal observations on study days 7 and 14.

At termination, the rats were euthanized by carbon dioxide asphyxiation. The major organ systems of the cranial, thoracic and abdominal cavaties were examined for all animals.

Results:

Value: $LD_{50} > 2000$ mg/kg

Number of deaths at each dose level: There were no deaths during the study.

Remarks: Nine animals had dried red material around the eye(s) and/or mouth and or/nose on the day of dosing. Urogenital staining (described as wet or dried yellow) was present for seven animals. Two rats had soft stool. These findings were considered unrelated to the test material, as they are often noted for rats that have been bandaged/collared. There were no other clinical findings. All animals appeared normal by day 2 and throughout the remainder of the observation period.

The test material induced very slight to slight erythema and edema along with desquamation on all rats. There were no other dermal findings. All erythema and edema completely subsided by days 11 and 7, respectively. Desquamation persisted through study termination (day 14) on two sites.

There were no remarkable changes or differences in body weights. One male had a dilated renal pelvis (right) at the scheduled necropsy. There were no other gross necropsy findings for all examined tissues.

The LD50 and the NOEL for systemic toxicity of tridecene were found to be greater than 2000 mg/kg.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

Reference: WIL Research Laboratories, Inc. (1995) Acute Dermal Toxicity Study of NEODENE®13 Internal Olefin in Albino Rats; Performed for Shell Chemical Co. (unpublished report).

(3) Test Substance

Identity (purity): CAS No. 68526-58-9, Alkenes, C11-13, C12 rich

Method

Method/guideline:	NA
Type (test type):	LD50
GLP:	Pre-GLP
Year:	1961
Species/Strain:	Albino rabbits
Sex:	Males and females
No. of animals per sex per dose:	2
Vehicle:	NA
Route of administration:	Dermal

Test Conditions: Age of the test animals was not reported. Body weights ranged from 1.3 to 2.2 kg at initiation of the study. Groups of animals were exposed to the test substance in single exposures to concentrations of 77.4, 245, 774, and 2446 mg/kg. Undiluted test material was applied to clipped, intact abdominal skin under rubber dental damming. For the purpose of this study, the test material was considered to be free of impurities. The trunks of the animals were wrapped securely with adhesive binder to prevent ingestion of the test substance. Following the 24-hour exposure period, the binder was removed and the exposed area was sponged with warm water to remove residue. Animals were observed for gross signs of irritation and systemic toxicity daily for 14 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually. Tissue samples were taken from animals at the 774 and 2446 mg/kg dose levels. No mortality occurred; therefore, statistical analysis of the data was not warranted.

Results:

Value:	LD_{50} > 2446 mg/kg
Number of deaths at each dose level:	No mortalities were observed at any dose tested.
Remarks:	One animal in the 245 mg/kg dose group had diarrhea on the last day of the study and a net loss of weight. The remaining animals exhibited normal appearance and behavior throughout the entire study and showed normal body weight gain. One animal in the 774 mg/kg and two animals in the 2446 mgl/kg dose groups had parasitic infections in the liver. No other abnormalities were observed at necropsy. Upon removal of the binders, the exposed skin showed slight erythema. Three of the high dose animals displayed slight edema, which subsided within 48 hours. By 48 hours, low dose animals showed no signs of irritation. Erythema in the high dose animals completely subsided by the third day. By Day 12, all signs of irritation had completely cleared in all of the animals with the exception of slight desquamation in one high dose animal. Alkenes, C11-13, C12-rich have a low order of acute dermal toxicity.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
Reference:	Hazleton Laboratories, Inc. (1961) Acute Oral Administratio-- - Rats, Acute Dermal Applicatio-- - Rabbits, Acute Eye Applicatio-- - Rabbits, Acute Inhalation Exposur-- - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co. (unpublished report).

(4) Test Substance

Identity (purity):	CAS No. 112-41-4, 1-Dodecene (Alpha Olefin C12)

Method

Method/guideline:	No data
Type *(test type):*	LD50
GLP:	Pre-GLP
Year:	1976
Species/Strain:	Rabbit/New Zealand White
Sex:	Not reported
No. of animals	

per sex per dose:	4
Vehicle:	None
Route of administration:	Dermal
Test Conditions:	1-Dodecene, neat, at 10 g/kg body weight was placed under a plastic sleeve wrapped around the clipped trunks of two intact and two abraded rabbits (2.3-3.0 kg). The material was allowed to remain in contact with the skin for 24 hours. The animals were observed for 14 days after removal of the sleeves.
Results:	One out of the four rabbits dies on the 7th day of observation. All other rabbits were gaining weight normally. There was very slight erythema on the first day of observations at the application site.
Value:	LD50 > 10 g/kg
Number of deaths at each dose level	1/4 at 10 g/kg body weight
Reliability:	(2) Reliable with restrictions: Incomplete reporting of experimental details.
References:	Carter, G. (1976) A report on the acute toxicity of Alpha Olefin C12, Ethyl Corporation (unpublished report).
Other:	This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

(5) Test Substance

Identity (purity):	C12-16 Alpha Olefin Fraction (GULFTENE 12-16)
Remarks	Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

Method

Method/guideline:	U.S. Federal Hazardous Substances Labeling Act
Type (test type):	LD50
GLP:	Pre-GLP
Year:	1967
Species/Strain:	Albino rabbits
Sex:	Males
No. of animals per sex per dose:	4

Vehicle: NA

Route of administration: Dermal

Test Conditions: Two groups of 4 rabbits (weighing between 2.3 and 3.0 kg) were used (treated and control). Prior to dosing, the animals were clipped free of hair over the entire trunk area. The skin of two animals from each group was abraded by making longitudinal epidermal abrasions spaced about 2-3 cm apart over the area to be exposed. Surgical gauze was wrapped around the animal and covered with an impervious plastic film. The animals in the treated group then received a dose of 10 g/kg test substance introduced under the plastic film. Following dosing, the animals were immobilized in stocks for 24 hr, after which the covering and excess material were removed and the skin examined for gross changes. Animals were weighed on Days 1-4, and on Days 7 and 14. Animals were observed for 14 days and then sacrificed and autopsied.

Results:

Value: $LD_{50} > 10$ g/kg

Number of deaths at each dose level: No mortalities that were related to exposure to test substance. One control animal died from pneumonia on Day 2.

Remarks: There were no signs suggestive of systemic toxicity. The skins of animals became very taut, dry and scaly, with no regrowth of hair in the clipped areas and a loss of hair from areas which became wet with the test substance. Autopsy showed no gross signs of damage to internal organs. Slight signs of pneumonia were observed in both treated and control animals. All treated animals showed weight loss on Days 1-7:

	% Weight Loss					
	Day 1	Day 2	Day 3	Day 4	Day 7	Day 14
C12-16	-9	-9	-4	-5	-4	0
Control	0	+2	+2	+3	+1	+4

Reliability: (2) Reliable with restrictions: Details of procedures are not available, individual animal data is not available, and animals appeared to have pneumonia.

Reference: Rinehart, W.E. (1967) Toxicological Studies on Several Alpha Olefins, for Gulf Research and Development Company (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

D. Acute toxicity, other routes

No data available

5.3 Corrosiveness/Irritation

A. Skin Irritation/Corrosion)

(1) Test Substance

Identity (purity): CAS No. 68526-58-9, Alkenes, C11-13, C12 rich

Method

Method/guideline:	NA
Type (test type):	Dermal irritation
GLP:	Pre-GLP
Year:	1961
Species/Strain:	Albino rabbits
Sex:	Males and females
No. of animals per sex per dose:	2
Vehicle:	NA
Route of administration:	Dermal

Test Conditions: Groups of animals were exposed to the test substance in single exposures to concentrations of 77.4, 245, 774, and 2446 mg/kg. Undiluted test material was applied to clipped, intact abdominal skin under rubber dental damming. The trunks of the animals were wrapped securely with adhesive binder to prevent ingestion of the test substance. Following the 24-hour exposure period, the binder was removed and the exposed area was sponged with warm water to remove residue. Animals were observed for gross signs of irritation and systemic toxicity daily for 14 days. Following the post-exposure observation period, animals were weighed, sacrificed and necropsied. Throughout the study, food and water were available at all times and animals were housed individually.

Age of the test animals was not reported. Body weights ranged from 1.3 to 2.2 kg at initiation of the study.

Results:

Number of deaths at each dose level: No mortalities were observed at any dose tested.

	Remarks:	Upon removal of the binders, the exposed skin showed slight erythema. Three of the high dose animals displayed slight edema, which subsided within 48 hours. By 48 hours, low dose animals showed no signs of irritation. Erythema in the high dose animals completely subsided by the third day. By Day 12, all signs of irritation had completely cleared in all of the animals with the exception of slight desquamation in one high dose animal.
	Reliability:	(1) Reliable without restrictions; however, exposure was more severe than recommended by current testing guidelines (i.e., current guidelines recommend semi-occlusive exposures for 4 hours)
	Reference:	Hazleton Laboratories, Inc. (1961) Acute Oral Administration - Rats, Acute Dermal Application - Rabbits, Acute Eye Application - Rabbits, Acute Inhalation Exposure - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co. (unpublished report).
(2)	**Test Substance:**	CAS No. 112-41-4, 1-Dodecene (95%, GULFTENE 12)
	pH:	Not applicable
	Method:	OECD 404
	Test Type:	in vivo
	GLP:	Yes
	Year:	1995
	Test Conditions	
	Species:	Rabbits
	Strain:	New Zealand White
	Cell type:	
	Sex:	Male and female
	Number of animals per sex per dose:	5 males and 1 female
	Total dose:	0.5 ml
	Vehicle:	None
	Exposure time period:	4 hrs
	Grading scale:	Draize
	Method Remarks:	At the start of the study, the animals weighed 2.48 to 2.84 kg and were approximately 12 to 20 weeks old. One-half ml undiluted material was applied to the unabraded skin on the shaved backs of 6 rabbits, under a semi-occluded dressing (cotton gauze patch placed in position with a strip of porous tape; trunk wrapped in an elasticated corset [TUBIGRIP]). A contralateral area of untreated

skin was identified to serve as the control against which the reactions of the treated site were evaluated. Four hours after application, the corset and patches were removed and residual test material was removed by swabbing with cotton wool soaked in 74% Industrial Methylated Spirits. The control sites were similarly swabbed. Scores were made for erythema and edema at 0.5, 24, 48, 72 and 96 hr after removal of patches, and at 7 and 14 days after initiation of exposure.

Results: All animals gained weight during the study. Well-defined erythema was noted at all treated skin sties at the 30-min, 24-hr and 48-hr observations. Well-defined erythema persisted at 3 treated sites at the 72-hr observation and at 2 sites at the 96-hr observation. Moderate to severe erythema was noted at 3 treated sites at the 72-hr observation and at 4 sites at the 96-hr observation. Very slight erythema was apparent at 4 treated sites at the 7-day observation. Crust formation was noted at 5 treated sites at the 7-day observation and at all treated sites at the 14-day observation. Crust formation was considered to be a reversible effect. The reactions extended up to 6 cm beyond each treated skin site during the study.

Slight edema was noted at 2 treated skin sites, moderate edema at 2 sites and severe edema at 2 sites at the 30-min observation. Slight or moderate edema was apparent at all sites at the 24 and 48-hr observations. Slight edema was noted at all treated sites at the 72 and 96-hr observations.

The Draize primary irritation index was 4.67. The mean 24-72 hr scores for erythema and edema were 2.2 and 2.4, respectively.

Reliability: (1) Reliable without restrictions

Reference: Driscoll, R. (1996) Acute dermal irritation test in the rabbit with GULFTENE 12, Report 703/078. Conducted by Safepharm Laboratories Ltd. for Chevron Research and Technology Company (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

(3) **Test Substance:** CAS No. 25377-82-6, Tridecene, 100%, NEODENE 13 Internal Olefin

Method: TSCA Health Effects Test Guidelines, 40 CFR 798.4470, meeting OECD Guidelines, Section 404

Test Type: in vivo
GLP: Yes
Year: 1995

Test Conditions

Species:	Rabbits
Strain:	New Zealand White
Cell type:	
Sex:	Male and female
Number of animals per sex per dose:	3
Total dose:	0.5 ml
Vehicle:	None
Exposure time period:	4 hrs
Grading scale:	Draize

Method Remarks: At the start of the study, the young adult animals weighed 3.35 to 3.99 kg. One-half ml undiluted material was applied to the clipped, unabraded skin on the backs of 6 rabbits, under occlusive dressing. Each 0.5 milliliter dose was applied to an area of skin approximately 1 inch by 1 inch under a secured 2-ply gauze patch that was overwrapped with a gauze binder, occluded with plastic wrap and secured with Dermiform® tape. Plastic restraint collars were applied and remained on the animals for the duration of the exposure period. Four hours after application, the collars and bandages were removed and the sites wiped with disposable paper towels moistened with deionized water. The application sites were observed for erythema, edema and other dermal findings approximately 30-60 minutes and 24, 48, and 72 hours after patch removal and daily thereafter through day 21 if irritation persisted. In order to facilitate dermal observations, the application sites were clipped free of hair approximately one hour prior to collecting the 72 hour, day 10 and day 21 dermal scores.

Results: There were no deaths and no remarkable body weight changes during the study. The test material induced slight to moderate erythema and edema along with desquamation on all animals. All edema completely subsided by day 19 or earlier. There were no other dermal findings. Very slight to moderate erythema and desquamation persisted through day 21 (termination) for five and four of the six rabbits, respectively.

The Draize Primary Dermal Irritation Index (the mean of combined scores for erythema and edema at 1 hour, 24 hour, 48 hour and 72 hour) was calculated to be 3.5.

Reliability: (1) Reliable without restrictions

Reference: WIL Research Laboratories, Inc. (1995) Primary Dermal Irritation Study of NEODENE®13 Internal Olefin in Albino Rabbits; Performed for Shell Chemical Co. (unpublished report).

B. Eye Irritation/Corrosion

(1) Test Substance: C10-13 Internal Olefins (Shop Olefins 103 PQ 11), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

pH: Not applicable

Method:

Test Type: in vivo
GLP: No
Year: 1977

Test Conditions

Species: Albino rabbits
Strain: New Zealand White
Number of animals per dose: 4

Dose(s) used: 0.2 ml
Vehicle: None
Observation period: 7 days

Remarks: The conjuctival redness chemosis and discharge, corneal opacity and damage to the iris following the instillation of 0.2 ml undiluted olefin into the conjuctival sac of four rabbit eyes was scored using standard Draize scales.

Results: Animals were observed within 1-2 hours, after 1, 2, 3, and 7 days of application. Mean Draize score was 1.0 (out of 110) at 1 hour after exposure, 0.9 for day 1, 0.1 for day 2, and 0 at other points.

Reliability: (1) Reliable without restrictions

Reference: Cassidy, S.L., Clark, D.G. (1977) Toxicology of alpha olefins: Acute toxicity, skin and eye irritancy and skin sensitizing potential of alpha olefin 103 PQ 11. Sittingbourne, Shell Research Limited, TLGR.0.171.77 (unpublished report).

(2) Test Substance

Identity (purity): CAS No. 68526-55-6; Alkenes, C11-13, C12 rich

Method

Method/guideline: Not specified
Type *(test type):* Ocular irritation

GLP:	Pre-GLP
Year:	1961
Species/Strain:	Albino rabbits
Sex:	Males and females
No. of animals per dose:	9
Vehicle:	None
Route of administration:	Ocular

Test Conditions: The test material was administered as a single instillation of 0.1 ml into the lower conjunctival sac of the left eye of each animal. The untreated eye in each rabbit served as the control. The treated eyes of three animals were irrigated with 20 ml of water four seconds following instillation, while the treated eyes of the six remaining animals were not irrigated but were held closed for 30 seconds following instillation. Throughout the study, food and water were available at all times and animals were housed individually. Test animals weighed between 1.8 and 3.5kg at the start of the study. The age of the animals and the statistics used to evaluate the data were not reported. The general health of each rabbit was examined for irritation of the cornea, iris and conjunctiva at 1 and 4 hours and on days 1, 2, 3, 4 and 7. Ocular reactions were graded according to the Draize Standard Eye Irritation Grading Scale.

Results: Maximum total Draize score = 10

Remarks: There were no animal deaths prior to study termination. The animals exhibited normal appearance and behavior throughout the study and gained weight. The test material produced a very slight degree of irritation in the three irrigated eyes and in four of the non-irrigated eyes. The two remaining non-irrigated eyes showed no signs of irritation at any time during the study. At 24 hours and for the duration of the observation period, the treated eyes of all animals appeared normal.

Reliability: (1) Reliable without restrictions

References: Hazleton Laboratories, Inc. (1961) Acute Oral Administration - Rats, Acute Dermal Application - Rabbits, Acute Eye Application - Rabbits, Acute Inhalation Exposure - Mice, Rats, Guinea Pigs; Performed for Esso Research and Engineering Co. (unpublished report).

(3) **Test Substance:** CAS No. 112-41-4, 1-Dodecene (C12 alpha olefin)

pH: Not applicable

Method: No data

Test Type: in vivo
GLP: No
Year: No data

Test Conditions

Species: Albino rabbits
Strain: New Zealand White
Sex: Not reported
Number of animals per dose: 6
Dose(s) used: 0.1 ml (neat)
Vehicle: None
Observation period: 24 hrs, 48 hrs, 72, hrs and 7 days
Scoring method used: Draize

Results: Individual animal scores at 24 hours are listed in the table below.

Structure	Score Rabbit Number						Mean
	1	2	3	4	5	6	
Cornea	5	0	0	0	0	0	2.5/110
Iris	0	0	0	0	0	0	
Conjunctiva	2	2	0	2	4	0	

All remaining scores at 48 and 72 hours were zero.

Reliability: (2) Reliable with restrictions. Complete set of raw data not reported

Reference: Carter, G. (1976) A report on the acute toxicity of Alpha Olefin C12, Ethyl Corporation, August (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

5.4 Skin Sensitisation

A. Test Substance: C10-13 Internal Olefins (Shop Olefins 103 PQ 11), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method: Magnusson and Kligman
Test Type: challenge
GLP: No
Year: 1977

Test Conditions

Species:	Guinea pig
Strain:	P strain
Sex:	Male and female
Number of animals per sex per dose:	10 in test group; 5 each in control group
Route of administration:	Injection and Topical
Intradermal	
Induction conc.:	0.05%
Induction vehicle:	corn oil
Topical	
Induction conc.:	1.5%
Induction vehicle:	corn oil
Challenge conc.:	10%
Challenge vehicle:	corn oil

Method remarks:

A preliminary screen was carried out using groups of 2 male and 2 female guinea pigs to determine the concentrations of test material to be used for intradermal induction, topical induction and topical challenge.

Induction was accomplished in 2 stages, intradermal injection and a topical application. Two rows of 3 injections were made: 2 of 0.1 ml Freund's complete adjuvant (FCA), 2 of 0.1 ml test material in solvent (solvent), and 2 of 0.1 ml test material in 50:50 FCA/solvent. The injection sites were just within the boundary of a 4x4 cm shaved area.

One week after the intradermal injections the same area was clipped. A 4x4 cm patch of Whatman No. 3 filter paper was soaked in a solution of the test material, placed over the injection sites of the experimental animals and covered by overlapping plastic adhesive tape (Blendaderm). This was secured with elastic adhesive bandage (Poroplast). The dressing was left in place for 48 hours.

The challenge procedure was carried out 2 weeks after topical induction. Challenge was accomplished by topical application of the challenge solution of the test material to the flank of both test and control groups of animals. 3x3 cm area on the flank was clipped and shaved. A 2.5x2.5 cm patch of Whatman No. 3 filter paper was soaked in a solution of the test material, placed over the injection sites of the experimental animals and covered by overlapping plastic adhesive tape (Blendaderm). This was secured with elastic adhesive bandage (Poroplast). The dressing was left in place for 24 hours. Examination of the challenge site was immediately, 24 and 48 hours after removal of the dressing.

Results: Negative for sensitization

Results Remarks: Number of animals with skin reaction at challenge: 0/10

Number of animals with skin reaction in control group at challenge: 0/10.

Reliability: (1) Reliable without restrictions

Reference: Cassidy, S.L., Clark, D.G. (1977) Toxicology of alpha olefins: Acute toxicity, skin and eye irritancy and skin sensitizing potential of alpha olefin 103 PQ 11. Sittingbourne, Shell Research Limited, TLGR.0.171.77 (unpublished report).

B. Test Substance: C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

Remarks: Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

Method: Landsteiner technique
Test Type: challenge
GLP: No
Year: 1967

Test Conditions
Species: Albino guinea pig
Strain:
Sex: Males
Number of animals per sex per dose: 10

Route of administration: Topical

Induction conc.: 100% for test substance
Induction vehicle: None for test substance, 50% ethyl alcohol for positive control
Challenge conc.: 100% for test substance
Challenge vehicle: None for test substance, 50% ethyl alcohol for positive control
Grading system used: Not specified

Method remarks: Three groups of ten male albino guinea pigs weighing 300-350 g each were used. A positive control group was exposed to 0.5% chlorodinitrobenzene in 50% ethyl alcohol in water. A second group was exposed to 50% ethyl alcohol only. The other group received olefin test article. Test sites on the backs of the animals were clipped and light abrasions of the outer dermal layer were made with a needle. 0.1 ml test article was applied to the test sites from a dropper and rubbed into the skin with a glass rod, three times weekly for nine applications. Type of dressing was not specified. Observations for erythema and edema were made 24 hours after applications. After the ninth application, animals were rested for two weeks. They were then challenged with 0.1

ml of test article or 0.5% chlorodinitrobenzene in 50% ethanol-water (the ethanol control animals also received chlorodinitrobenzene).

Results: Animals treated with C12-16 Alpha Olefin Fraction were not sensitized

Grades: See Remarks

Remarks: Only slight erythema was seen in one animal exposed to the alpha olefin after the eighth application and in two animals after the ninth application; no edema was seen. Animals exposed to alcohol showed no reactions at any time point. The positive control animals showed moderate erythema in all animals after the third application, and mild edema in half the animals after the seventh application. During the 2-wk rest interval, signs of erythema and edema disappeared from all animals.

Twenty-four hours after the challenge, alpha olefin treated animals showed no response. The positive control group showed severe erythema in all animals. The animals pre-treated with alcohol given chlorodinitrobenzene as a challenge for comparison with the positive control group showed only a very slight erythema in 2 animals.

Reliability: (1) Reliable without restrictions

Reference: Rinehart, W.E. (1967) Toxicological Studies of Several Alpha Olefins Conducted by Department of Occupational Medicine, University of Pittsburgh, Pittsburgh, Pennsylvania, for Gulf Research and Development Company (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

5.5 Repeated Dose Toxicity

Test Substance

Identity (purity): C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

Remarks: Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

Method

Method/guideline:
Test type: Subacute toxicity
GLP: Yes
Year: 1983
Species: Rat

Strain:	Fischer 344
Route of Administration:	Dermal
Duration of test:	2 weeks
Doses:	0, 1.0, and 2.0 g/kg/day
Sex:	Males and females
Exposure period:	2 weeks
Frequency of treatment:	Once daily for 9 doses over 2-wk period
Control group and treatment:	Concurrent vehicle control (5 M, 5 F, corn oil)
Post exposure observation period:	None
Statistical methods:	Organ weights: Bartlett's test and one-way analysis of variance; if the Bartlett's test indicated the data were homogeneous, Dunnett's test was also performed; if the Bartlett's test indicated the data were non-homogeneous, a modified t-test was performed. Histopath: Kolmogorov-Smirnov Two-Tail Test (0.05 level of significance)

Test Conditions:

Animals were approximately 7 weeks of age and weighing 90-120 g at study initiation. Prior to treatment, the backs of all animals were clipped free of hair. To prevent ingestion of the test substance, each animal was fitted with an Elizabethan collar. The collar remained on the animals until removal of residual test/control substance. Dermal doses of 2.0 g/kg (undiluted) or 1.0 g/kg (diluted 1:1 with corn oil prepared weekly) of GULFTENE 12-16 were administered to groups of 5 males and 5 female Fischer 344 rats, in 9 daily doses over a 2-wk period. An equivalent volume of the vehicle was administered to the control group. The treated area was approximately 10% of the body surface. Approximately 6 hrs following each application, residual test substance was wiped from the application site. Parameters evaluated for treatment-related effects included survival; body weight (weekly); food consumption (weekly); appearance and behavior (at least once daily on dosing days); dermal reaction (according to the method of Draize on each dosing day prior to dosing and after removal of residual material); hematology (blood samples collected via orbital sinus) and clinical chemistry (collected prior to treatment and necropsy); organ weights, organ weight ratios relative to body and brain weights (liver, brain, spleen, heart, kidney, testes); gross pathology, and microscopic pathology (control and high-dose animals only: lungs, skin, liver, brain, spleen, heart, kidney, testes, ovaries). All animals were sacrificed approximately 24 hrs after the ninth treatment by inhalation of methoxyflurane.

Results

NOAEL (NOEL): NOAEL: 1g/kg/day (systemic) [By summary author – study authors did not declare a NOAEL]
LOAEL: 2 g/kg/day (systemic) [By summary author – study authors did not declare a NOAEL]

Remarks:

All animals survived to the end of the study and no moribund animals were observed during the study.

Repeated application of undiluted GULFTENE 12-16 at 2.0 g/kg produced severe erythema (beet redness) to slight eschar formation (injuries in depth) and slight edema (edges of area well defined by definite raising) in all animals. Dermal reactions increased in severity with the number of applications. In all animals, slight to moderate desquamation was detected after the second treatment and persisted until the end of treatment. Slight to moderate hair loss was detected in 8/10 animals after the eighth treatment. Fissuring was also noted in 4 female animals after 6 treatments.

When GULFTENE 12-16 was administered at a 1.0 g/kg level, 2 males exhibited very slight erythema (barely perceptible) after 6 treatments and a third male after seven treatments. In one of the 3, the intensity of the erythema increased to slight and a pinpoint spot of eschar was observed after the seventh treatment. All reactions persisted throughout the study period. No edema or other reactions were noted.

In comparison to controls, depressed body weight gains were observed in the 2.0 g/kg group but not in the 1.0 g/kg group. In the 2.0 g/kg group, means for males and females increased by 25.6 g and 22.8 g, respectively, while means for control males and females increased by 52.3 g and 28.8 g, respectively, over the study period.

In the 2.0 g/kg group, the decreases in bodyweight were associated with decreases in the absolute weights of most organ systems (mean, treated vs control):

- liver: males = 6.35 g vs 7.99 g [p = 0.01]
- brain: females = 1.56 g vs 1.60 g [p = 0.05]
- spleen: males = 0.39 g vs 0.43 g [p = 0.05]
- heart: males = 0.55 g vs 0.65 g [p = 0.01]
- kidney, left: males = 0.59 g vs 0.64 g [p = 0.05]
- kidney, right: not sig. different from control
- testes: not sig. diff. from control

In the 2.0 g/kg group, the changes in body and organ weights resulted in statistically significant differences in the relative weight ratios for several organs (mean ratio in treated vs control):

- brain: males = 1.24 vs 1.04 [p = 0.01]
- spleen: males = 0.29 vs 0.27 [p = 0.01] and females = 0.32 vs 0.29 [p = 0.01]
- kidney, left: males = 0.45 vs 0.40 [p = 0.01] and females = 0.47 vs 0.42
- kidney, right: males = 0.45 vs 0.39 [p = 0.01] and females = 0.47 vs 0.43 [p =0.05]
- testes: not sig. diff. from control

In the 2.0 g/kg group, the changes in body and organ weights resulted in statistically significant differences in the organ/brain weight ratios (mean ratio in treated vs control):

- liver: males = 3.97 vs 4.78 [p = 0.05]
- heart: males = 0.33 vs 0.39 [p = 0.05]
- kidney, left: males = 0.36 vs 0.38 [p = 0.05]

No treatment related effects were noted for food consumption, clinical signs (other than dermal reactions), hematology, and clinical chemistry. Treatment was associated with histological changes in the skin at the point of application in all animals. There were no other microscopic changes seen that could be associated with the test substance.

Study authors concluded that, under conditions of the study, repeated dermal applications of GULFTENE 12-16 at 2.0 g/kg, but not at 1.0 g/kg, caused severe skin reactions and depressed body weight gains.

Reliability: (1) Reliable without restrictions.

References: Gulf Life Sciences Center (1983) Two-Week Repeated Dose Toxicity Study in Rats Using GULFTENE 12-16, Project No. 82-059. Conducted for Gulf Oil Chemicals Company (unpublished report).

5.6 Genetic Toxicity *in vitro*

A. Gene Mutation

(1) **Test Substance:** C10-13 Internal Olefins (Shop Olefins 103), linear

Remarks: Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method/guideline:	
Type:	in-vitro bacterial reverse mutation – Ames Assay
System of testing:	bacterial
GLP:	No
Year:	1983
Species/Strain:	*Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538, and *Escherichia coli* WP_2 or WP_2 uvrA
Metabolic activation:	With and without S9 fraction from induced rat livers
Concentrations tested:	31.25, 62.5, 125, 250, 500, 1000, 2000 and 4000 µg/plate
Statistical Methods:	The mean and SD of the colony counts from cultures derived from each flask were computed by standard methods.

Test Conditions: 20 µl volumes of solutions of Olefin 103 PQ/11 in ethanol/Tween 80 (1.5625, 3.125. 6.25. 12.5, 50, 100 mg/ml) or 40 ul of 100 mg/ml were added to top agar mix to give final solutions of 31.25, 62.5, 125, 250, 500, 1000, 2000 and 4000 µg/plate both in the presence and in the absence of rat liver S9 fractions. The cultures were incubated at 37°C for 48-72 hours before the revertant colonies were counted. The activity of the S9 mix and the sensitivities of the strains TA1538, TA98 and TA100 were monitored by treating cultures with a known positive control compound, benzo (a) pyrene, with requires metabolic activation before it is able to induce gene mutation. The sensitivity of TA1537 was monitored by the indirect mutagen, neutral red; the sensitivities of *E. coli* WP_2 or WP_2 uvrA pkm 101 and TA1535 were monitored by testing with the direct-acting mutagens, potassium dichromate or sodium azide, respectively.

Results

Cytotoxic conc.: No cytotoxicity observed
Genotoxic effects: Negative with and without metabolic activation

Remarks: The test material did not lead to an increase in reverse mutation frequency in any strain. No visible precipitation of the test compound was observed in the top agar overlay. Microscopic examination of the background lawn in the plate incorporation assay showed no reduction in growth in any of the strains tested. All positive and negative controls responded in a manner consistent with data from previous assays. The addition of Olefin 103 PQ/11 at amount up to 4000 µg per plate to agar layer cultures of *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538, and *Escherichia coli* WP_2 or WP_2 uvrA did not lead to an increase in the reverse gene mutation frequency in any of the strains either in the presence or absence of rat liver S9 fractions.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint.

References: Brooks, TM, Clare, MG, Wiggins, DE (1983) Toxicity studies with detergents: Genotoxicity studies with Olefin 103 PQ/11 (Cracked Urea Wax Olefin). Shell Research Limited, SBGR.83.299 (unpublished report).

(2) Test Substance

Identity (*purity*): CAS No. 112-41-4, 1-Dodecene (C12 alpha olefin)

Method

Method/guideline:	No data
Type:	in-vitro bacterial reverse mutation – Ames Assay
System of testing:	bacterial
GLP:	No
Year:	1980
Species/Strain:	*Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538, and *Escherichia coli* WP_2 or WP_2 uvrA
Metabolic activation:	With and without S9 fraction from induced rat livers
Concentrations tested:	0, 0.2, 2.0, 20, 200 and 2000 µg/plate
Statistical Methods:	The mean and SD of the colony counts from cultures derived from each flask were computed by standard methods.

Test Conditions: 20 ul volumes of solutions of Olefin 103 PQ/11 in ethanol/Tween 80 (1.5625, 3.125. 6.25, 12.5, 50, 100 mg/ml) or 40 ul of 100 mg/ml were added to top agar mix to give final solutions of 31.25, 62.5, 125, 250, 500, 1000, 2000 and 4000 µg/plate both in the presence and in the absence of rat liver S9 fractions. The cultures were incubated at 37°C for 48-72 hours before the revertant colonies were counted.

Results

Cytotoxic conc.:	No cytotoxicity observed
Genotoxic effects:	Negative with and without metabolic activation

Remarks: The test material did not lead to an increase in reverse mutation frequency in any strain. The test material did not lead to an increase in reverse mutation frequency in any strain. No visible precipitation of the test compound was observed in the top agar overlay. Microscopic examination of the background lawn in the plate incorporation assay showed no reduction in growth in any of the strains tested. All positive and negative controls responded in a manner consistent with data from previous assays

The addition of the test material at amounts up to 4000 ug per plate to agar layer cultures of *Salmonella typhimurium* TA98, TA100, TA1535, TA1537, TA1538, and *Escherichia coli* WP_2 or WP_2 uvrA did not lead to an increase in the reverse gene mutation frequency in any of t he strains either in the presence or absence of rat liver S9 fractions.

The activity of the S9 mix and the sensitivities of the strains TA1538, TA98 and TA100 were monitored by treating cultures with a known positive control compound, benzo (a) pyrene, with requires metabolic activation before it is able to induce gene mutation. The sensitivity of TA1537 was monitored by the indirect mutagen, neutral red; the sensitivities of *E. coli* WP_2 or WP_2 uvrA pkm 101 and TA1535 were monitored by testing with the direct-acting mutagens potassium dichromate or sodium azide respectively.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint.

References: Dean, B.J. (1980) Toxicity studies with detergent intermediates: In vitro genotoxicity studies with Shop process components. Shell Research Limited, TLGR.80.074 (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

(3) **Test Substance**

Identity (*purity*): C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

Remarks: Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

Method

Method/guideline:	Equivalent to OECD 476 except that a confirmatory assay was not conducted
Type:	Mammalian cell gene mutation assay
System of testing:	non-bacterial
GLP:	Yes
Year:	1982
Species/Strain:	Chinese Hamster Ovary Cell (CHO-K1) received from Dr. J.P. O'Neill, Oak Ridge National Laboratories, Oak Ridge, Tennessee.
Metabolic activation:	With and without S9 fraction of livers from rats pretreated with Aroclor 1254; protein concentration = 10 mg/ml; 0.3 ml S9/flask
Concentrations tested:	128, 512, 1024, and 2048 ug/mL; Doses were based on a pre-test for toxicity
Statistical Methods:	The mean and SD of the colony counts from cultures derived from each flask were computed by standard methods. Relative Survival: mean colony count in treated cultures ÷ by mean count in control cultures. Cloning Efficiency: mean colony count in each group ÷ by number of cells seeded per plate. Frequency of Mutant Colonies: ratio of total colony counts in the mutagenicity plates over total colony counts in the viability plates; group mean calculated. The frequency of mutant colonies per million clonable cells in the treated and vehicle control cultures were compared using Student's t test. A test was considered positive if there was a significant increase in mutant colonies at any dose level and a dose-related response.

Test Conditions:

The test substance was emulsified with 10% F68 Pluronic® Polyol in water and subsequently diluted with medium to a dosing preparation of 6% F68. Water was the vehicle for the direct acting positive control (ethylmethanesulfonate, 100 µg/ml in culture flask). DMSO was the vehicle for positive control cultures requiring metabolic activation (benzo(a)pyrene, 4 µg/ml in culture flask).

Cells were maintained in 5 ml Ham's F12 Medium (no hypoxanthine) with 5% dialyzed heat-inactivated newborn calf serum. During treatment the serum was omitted, HEPES buffer and antibiotic were included and the volume limited to 3 ml/flask. Where indicated, activating enzymes were included. After treatment, cultures were maintained in Ham's F12 (no hypoxanthine) with 5% dialyzed heat-inactivated newborn calf serum and antibiotics. For selection of mutant cells, 10^{-5} M 6-thioguanine was included. Incubation was in a CO_2 enriched (5%) humidified (95%) atmosphere at 37.5°C except that during exposure the sealed cultures were placed in a shaker incubator at 37°C.

RANGEFINDING: Approx. 5 x 10^5 cells seeded to each of 2 flasks/treatment (1 w/S9; 1 w/o S9); exposed to test substance at 4 – 2,048 µg/ml for 5 hrs on Day 2; on Day 3 tripsinized and counted with a Coulter Model ZB cell counter and subcultured (200 cells transferred to each of 3 60 mm culture dishes); incubated to Day 10/11; fixed in methanol and stained with Giemsa; colonies counted visually or with Artek Model 981 counter.

MUTAGENICITY: Each dose group was composed of 6 flasks, 3 w/S9, except that the vehicle group contained 12 flasks, 6 w/S9. The concentrations of test substance were 4, 16, 128, 512, 1024, and 2048 µg/ml. Control cultures received F68, medium, S9 mix or F68 with positive control. Sufficient cells were seeded to give approx. 1 million cells on Day 2 and exposed to test substance for 5 hrs on Day 2; on Day 3 all cultures were checked for evidence of cytotoxicity, and those showing excessive toxicity terminated. VIABILITY: 4 dose levels were subcultured (200 cells were transferred to each of 4 60 mm viability plates) and incubated to Day 10/11, fixed in methanol and stained with Giemsa, and colonies counted visually or with Artek Model 981 counter. MUTAGENICITY: 10^5-10^6 cells seeded to 100 mm dish on Day 3 for expression; subcultured 3 times, the last on Day 10/11; 200 cells seeded to each of 4 viability plates as above, and 2 x 10^5 cells seeded to each of 5 mutagenicity plates in selective medium; cultures incubated undisturbed until Day 16/18, when they were fixed and stained.

Results

Cytotoxic conc.: ≥ 1024 µg/ml
Genotoxic effects: Negative with and without metabolic activation

Remarks: RANGEFINDING: Some toxicity was evident at 2048 µg/mL without activation [cell count after treatment (x 10^5/ml) = 6.6, 6.6, 6.1, 6.4, 6.2, 5.8, 2.8 for concentrations of GULFTENE 12-16 of 0 (vehicle), 64, 128, 256, 512, 1024, and 2048 µg/ml, respectively]; and with activation [cell count after treatment (x 10^5/ml) = 4.1, 4.0, 2.9, 3.4, 3.4, 3.5, 2.9, 2.0 for concentrations of GULFTENE 12-16 of 0 (vehicle), 32, 64, 128, 256, 512, 1024, and 2048 µg/ml, respectively]. Toxicity was within acceptable limits.

DEFINITIVE TEST: A toxic effect was noted in that there were insufficient cells after treatment to subculture at 1 X 10^6 per dish at the 1024 and 2048 levels without activation and that cultures with activation also showed immediate toxicity at those levels [cell counts after treatment (x 10^5/ml) = 5.1, 5.1, 4.4, 2.8, and 2.1 at concentrations of 0 (vehicle), 128, 512, 1024, and 2048 µg/ml, respectively]. Colony counts after subculture showed that cells which were used to determine the mutagenic effect were able to grow and had recovered from the initial toxic effect. Cloning Efficiency after treatment = 64% and 56% at 2048 µg/ml (w/o and w/S9, respectively). Relative Survival after treatment = 83% and 68% at 2048 µg/ml (w/o and w/S9, respectively). Cloning Efficiency after expression = 82% and 86% at 2048 µg/ml (w/o and w/S9, respectively). Relative Survival after expression = 97% and 100% at 2048 µg/ml (w/o and w/S9, respectively). The frequency of mutant colonies was increased to expected values in the two positive control groups indicating the assay was functional. There were no increases over control in frequency of mutant colonies when cultures were treated with test article.

Reliability: (2) Reliable with restrictions: Confirmatory assay was not conducted.

References: Gulf Life Sciences Center, Pittsburgh, Pennsylvania (1983) CHO/HGPRT Test: GULFTENE 12-16, Project 82-102. Conducted for Gulf Oil Chemicals Company (unpublished study).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

B. Chromosomal Aberration

(1) Test Substance: C10-13 Internal Olefins (Shop Olefins 103), linear

Remarks:	Blend of CAS No. 25339-53-1 (C_{10} = 6-12%); CAS No. 28761-27-5 (C_{11} = 27-45%); CAS No. 25378-22-7 (C_{12} = 37-47%); CAS No. 25377-82-6 (C_{13} = 8-17%)

Method

Method/guideline:	
Type:	in-vitro rat liver cell chromosome aberration assay
System of testing:	non-bacterial
GLP:	No
Year:	1983
Type of cell used:	Rat liver RL1 cells
Metabolic activation:	No
Concentrations tested:	up to 500 µg/ml
Statistical Methods:	

Test Conditions: The range of concentrations of the test compound to be used to assess the cloning efficiency was determined from the results of the initial assay. For each concentration, including the solvent control, three 9 cm diameter Petri dishes were used. Five hundred RL4 cells were added to each dish and cells were incubated in 10 ml tissue culture medium at 37°C in a humidified atmosphere containing 5% CO2. Twenty-four hours after adding the cells, the medium was replaced with medium containing the compound or solvent, which was replaced with fresh medium after 24 hours exposure. Five days later the cells were fixed and stained. Colonies containing at least 50 cells were counted. The concentration of the test compound that reduced the number of colonies to an average of approximately 50% of those on the dishes exposed to solvent only was used as the highest concentration in the chromosome assay.

Results

Cytotoxic conc.:	No cytotoxicity observed
Genotoxic effects:	Negative

Remarks: There was no significant increase in the frequency of chromatid gaps, chromatid breaks or total chromatid aberrations in rat liver (RL4) cell cultures exposed to Olefin 103 PQ/11 at concentrations up to 25 ug per ml. All positive and negative controls responded in a manner consistent with data from previous assays.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Dean, B.J. (1980) Toxicity studies with detergent intermediates: In vitro genotoxicity studies with Shop process components. Shell Research Limited, TLGR.80.074 (unpublished report).

(2) **Test Substance**

Identity (*purity*): CAS No. 112-41-4, 1-Dodecene

Method

Method/guideline:	No data
Type:	in-vitro rat liver cell chromosome aberration assay
System of testing:	non-bacterial
GLP:	Yes
Year:	No data
Type of cell used:	Rat liver RL1 cells
Metabolic activation:	No
Concentrations tested:	up to 500 μg/ml
Statistical Methods:	No data

Test Conditions: The range of concentrations of the test compound to be used to assess the cloning efficiency was determined from the results of the initial assay. For each concentration, including the solvent control, three 9 cm diameter Petri dishes were used. Five hundred RL4 cells were added to each dish and cells were incubated in 10 ml tissue culture medium at 37°C in a humidified atmosphere containing 5% CO2. Twenty-four hours after adding the cells, the medium was replaced with medium containing the compound or solvent, which was replaced with fresh medium after 24 hours exposure. Five days later the cells were fixed and stained. Colonies containing at least 50 cells were counted. The concentration of the test compound that reduced the number of colonies to an average of approximately 50% of those on the dishes exposed to solvent only was used as the highest concentration in the chromosome assay.

Results

Cytotoxic conc.:	No cytotoxicity observed
Genotoxic effects:	Negative

Remarks: A single exchange figure was observed but this occurred on one untreated control culture. Since no dose related increase in frequency of chromatid gaps, chromatid breaks or total chromatid aberrations were observed, it is concluded that alpha C_{12} product did not induce a direct cytogenetic effect in cultured RL_1 cells.

There was no significant increase in the frequency of chromatid gaps, chromatid breaks or total chromatid aberrations in rat liver (RL4) cell cultures exposed to the test material at concentrations up to 25 ug per ml.

All positive and negative controls responded in a manner consistent with data from previous assays.

Reliability: (1) Reliable without restrictions

Flag: Key study for SIDS endpoint

References: Dean, B.J. (1980) Toxicity studies with detergent intermediates: In vitro genotoxicity studies with Shop process components. Shell Research Limited, TLGR.80.074 (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

C. Other Genetic Effects

(1) Test Substance

Identity (*purity*): C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

Remarks: Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

Method

Method/guideline:	OECD 482 except that independent repeat was not conducted
Type:	In-vitro unscheduled DNA synthesis
System of testing:	Non-bacterial
GLP:	Yes
Year:	1984
Cell line:	Primary rat hepatocytes
Metabolic activation:	None
Concentrations tested:	Rangefinding experiment: 8, 16, 32, 64, 128, 256, 512, 1024, 2048 and 5000 µg/ml UDS experiment: 100, 1000, 2000 and 4000 µg/ml
Statistical Methods:	The test substance was considered positive for unscheduled DNA synthesis (UDS) when the mean net nuclear grain count at any treatment level exceeded that of the concurrent negative control by at least 6 grains per nucleus, and the value for the negative control did not exceed 5. A dose response was not needed.

Test Conditions: Primary cultures of hepatocytes from livers of freshly perfused F344 rats were exposed to the test substance in the presence of ^{3}H-thymidine. Cytotoxicity was evaluated in a separate assay and

used as a basis for dosage selection. The occurrence of UDS was visualized autoradiographically and quantified with the aid of microscopy.

A 10% solution of Pluronic® F68 Polyol in water was used to emulsify the test substance. This was diluted with medium so that the concentration of F68 in the dosing preparations was 3.5% . Dosing preparations were added to the cultures in aliquots of 30 or 50 ul. This produced a culture concentration of 0.035% F68. The positive control was 2-acetylaminofluorene (2-AAF) prepared using DMSO and Pluronic F68 Polyol and administered at 0.2 ug/ml 2-AAF in the final culture.

The cells were grown in 3 ml (UDS) or 5 ml (rangefinding) Williams Medium E supplemented with 10% fetal bovine serum and insulin. Antibiotics were included. During the exposure period, 0.1M HEPES buffer, 2% by volume, and 0.1N HCL, 1% by volume, were present in the medium. The cells were cultured in plastic vessels. Incubation was in a carbon dioxide-enriched (5%), humidified atmosphere at 37°C. During the exposure period, cultures were sealed.

RANGEFINDING EXPERIMENT: In the rangefinding experiment, hepatocytes were harvested from one male rat aged 11 weeks and weighing 250 g. Two cultures each were prepared for the negative control, vehicle control and 10 levels of test substance. Approximately 1 x 10^5 cells/ml were seeded into each treatment culture and exposed to the test substance for 18 hours. The cells were then stained with trypan blue, fixed with formalin, and counted for viability determination. The culture vessel was taken as the experimental unit. The average number of viable cells per treatment group was determined. The relative viability was then calculated as the average number of viable cells in substance-treated cultures divided by that in the vehicle control cultures. For the evaluation of toxicity, at least 50% viability was desired. The final choice of treatment levels was based on the expectation that at least one level showed toxicity.

UDS EXPERIMENT: In the UDS experiment, hepatocytes were harvested from 1 male rat aged 13 weeks and weighing 270 g. Three cultures each were prepared for the negative control, vehicle control, positive control, and 4 levels of test substance. Approximately 1 x 10^5 cells/ml were seeded into each treatment culture and exposed to ^{3}H-thymidine and test substance for 18 hours. Cells growing on coverslips were rinsed, exposed to hypotonic solution, fixed, air dried and glued to microscope slides on Day 2. On Day 3, the slides were dipped in autoradiographic emulsion and stored in the dark at 2-8°C. Autoradiographs were developed, stained and coversliped on Day 13. The number of grains overlying each of 50 randomly selected nuclei per slide was counted microscopically. The

highest of 3 cytoplasmic grain counts per cell was subtracted to obtain the net nuclear grain count. The individual slide was taken as the experimental unit. The average net nuclear grain count per slide (sum of net nuclear grain counts divided by 50) was calculated and the mean net nuclear grain count (average net nuclear grain count per slide divided by 3) was determined for each treatment level.

Results

Cytotoxic conc.: 256 µg/ml

Genotoxic effects: Negative

Remarks: In the rangefinding experiment, GULFTENE 12-16 was toxic to primary hepatocytes beginning at 256 µg/ml where 74% relative viability was observed following an 18-hr exposure period. Cytotoxicity increased only slightly with increasing dose to 2048 µg/ml and then increased sharply at the highest dose tested, 5000 µg/ml, where a relative viability of 45.1% was observed. In the UDS experiment, both positive and negative controls gave the expected responses. No treatment level elicited a positive response for UDS.

Reliability: (2) Reliable with restrictions: Confirmatory assay not conducted

References: Gulf Life Sciences (1984) Hepatocyte Primary Culture/DNA Repair Test of GULFTENE12-16, project #2069 (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

(2) Test Substance

Identity (*purity*): C12-16 Alpha Olefin Fraction (GULFTENE 12-16)

Remarks: Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

Method

Method/guideline: Equivalent to US EPA TSCA 40 CFR 795.285 and ECC B21, except that a confirmatory assay was not conducted
Type: BALB/3T3 Transformation Test
System of testing: Non-bacterial
GLP: No

Year:	1983
Cell line:	Mouse embryo cells, BALB/3T3-A31-1-1
Metabolic activation:	None
Concentrations tested:	Rangefinding experiment: 8, 16, 32, 64, 128, 256, 512, 1024, 2048 and 5000 μg/ml Transformation experiment: 10, 20, 30 and 1500 μg/ml
Statistical Methods:	A test was considered positive if there were: 1) a two-fold increase in Type-III foci at the highest dose over that seen in vehicle control cultures, with or without a dose-related response or 2) a two-fold increase at two or more consecutive dose levels. Where vehicle control cultures have no Type-III foci, at least 2 foci would be needed for a dose level to be considered positive.

Test Conditions:

Cytotoxicity was evaluated in a separate assay and used as a basis for dosage selection.

A 10% solution of Pluronic® F68 Polyol in water was used to emulsify the test substance. This was diluted with medium so that the concentration of F68 in the dosing preparations was 3.5%. Dosing preparations were added to the cultures in aliquots of 50 μl. This produced a culture concentration of 0.035% F68. The positive control was 3-methylcholanthrene (3-MC) prepared using DMSO and Pluronic® F68 Polyol and administered at 1 μg/ml 3-MC in the final culture.

The cells were received from Dr. Takeo Kakunaga, National Cancer Institute, at Passage 14 after origination of the subclone. The cells were subcultured once, tested for presence of adventitious infectious agents and for capability to respond to known transforming agents, and frozen. Cultures used in testing were less than 4 additional passages from frozen stock. The cells were grown in 5 ml Eagle's Minimum Essential Medium supplemented with 10% heat-inactivated fetal calf serum. Antibiotics were included. Incubation was in a carbon dioxide-enriched (5%), humidified atmosphere at 37°C.

RANGEFINDING EXPERIMENT: Each treatment group (medium, vehicle, and 10 levels of test substance) consisted of two cultures. Approximately 1 x 10^4 cells were seeded into each treatment flask on Day 1. The cultures were exposed to the test substance for 2 days, beginning on Day 2, then trypsinized and counted on Day 4 with a Coulter Model ZB cell counter. The culture vessel was taken as the experimental unit. The average number of surviving cells per treatment group was determined. The relative survival was then calculated as the average number of surviving cells in substance-treated cultures divided by that in the vehicle control cultures. For the evaluation of toxicity, at least 20% survival was desired. The final choice of treatment levels was based on the expectation that at least one level showed toxicity.

TRANSFORMATION EXPERIMENT: Each group (medium control, vehicle control, positive control, and 4 levels of test substance) consisted of 15 flask cultures for transformation and 2 flask cultures for cloning. Transformation flasks were seeded with approximately 1 x 10^4 cells and cloning flasks with approximately 100 cells on Day 1. The cells were exposed to test substance for 2 days beginning on Day 2. The medium was changed on all cultures on Day 4. Cloning cultures were fixed and stained for colony counting on Day 8. Colonies (at least 50 cells) were counted visually and, where required, examined microscopically. The medium was changed weekly on all transformation flask cultures. Fixation and staining of flask cultures for focus counting and evaluation were on day 29. Foci were counted visually and examined microscopically to determine type.

The cloning efficiency was determined by dividing the average number of colonies (at least 50 cells) per flask by the number of cells seeded and converting to a percent. The relative cloning efficiency was determined by dividing the cloning efficiency for each treatment group by the cloning efficiency for the vehicle control, and converting to a percent. The transformation frequency for each group was the total number of Type III foci divided by the total number of flasks per group.

Results:

Cytotoxic conc.: Concentrations of >20 μg/ml were cytotoxic
Genotoxic effects: Negative

Remarks: In the rangefinding experiment, GULFTENE 12-16 was toxic to BALB/3T3 cells at 32 ug/ml when 16% viability was observed following a 2-day exposure period. Viability remained at this level up to a dose of 2048 μg/ml. At 5000 μg/ml, the relative viability was reduced to 1.3%.

In the transformation experiment, cloning efficiency was used as a measure of toxicity. Toxicity became evident at 20 μg/ml (27% relative cloning efficiency) and remained near this level through the highest dose tested, 1500 μg/ml.. The positive control gave the expected response. The negative controls were within acceptable limits for the test. No treatment level exceeded the medium controls for Type III foci. Under the conditions of the test, GULFTENE 12-16 was negative for cell transformation.

Reliability: (2) Reliable with restrictions: Confirmatory assay not conducted

References:

Goode, J.W. and Brecher, S. (1983) GULFTENE 12-16: BALB/3T3 transformation test, Project 2070. Sponsored by Gulf Life Sciences Institute, Pittsburg, PA (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

(3) Test Substance

Identity (*purity*): C11-12 Alpha Olefins (Blend not specified)

Remarks: Blend of CAS No. 821-95-4 (C_{11}) and CAS No. 112-41-4 (C_{12})

Method

Method/guideline:	
Type:	in-vitro mitotic gene conversion assay
System of testing:	non-bacterial
GLP:	Yes
Year:	1981
Species/Strain:	*Saccharomyces cerevisiae* JD1

Metabolic activation: With and without S9 fraction from induced rat livers

Concentrations tested: 0, 0.01, 0.1, 0.5, 1.0, and 5.0 mg/L

Statistical Methods: Reproducible values of greater than twice the control value are considered to indicate a mutagenic response.

Test Conditions: Number of replicates: 2 per concentration; Solvent: acetone; Positive control materials: cyclophosphamide (10 mg/ml) or 4-nitroquinoline-N-oxide (0.001 or 0.0001 mg/ml). Liquid suspension cultures of Saccharomyces cerevisiae JD1 were dosed with 20 µl (without S9 mix) or 25 µl (with S9 mix) of appropriate solutions or suspensions of C11-12 olefins to give final concentrations of 0.01, 0.1, 0.5, 1.0, and 5.0 mg/ml. After 18 hours incubation at 30°C the cultures were seeded onto the appropriate culture media plates for the selections of revertant colonies. After 3 days incubation at 30°C the numbers of revertant colonies on the plates were counted.

Results

Cytotoxic conc.:	No cytotoxicity observed
Genotoxic effects:	Negative with and without metabolic activation

Remarks: The addition of Olefin C_{11-12} to liquid suspension cultures of S. cerevisiae JD1, with or without the incorporation of rat liver S9 fraction, did not induce a consistent increase in mitotic gene conversion. The increases seen were not repeatable, nor dose-related and were therefore not considered to be an effect of the compound.

All positive and negative controls responded in a manner consistent with data from previous assays.

Reliability: (1) Reliable without restrictions

References: Brooks, T.M. (1982) Toxicity of detergents/higher olefins: In vitro genotoxicity studies on Shop products (olefins C11 – C12 and C13 – C14, olefin HE bleed and olefin intermediate recycle). Sittingbourne, Shell Research Limited, SBGR.81.325 (unpublished report).

Other: This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

5.7 Genetic Toxicity *in vivo*

Test Substance

Identity (purity):	C12-16 Alpha Olefin Fraction (GULFTENE 12-16)
Remarks	Blend of linear 1-dodecene (CAS No. 112-41-4), 1-tetradecene (CAS No. 1120-36-1), and 1-hexadecene (CAS No. 629-73-2). Composition of the blend was undefined in the report; analysis of other contemporary GULFTENE 12-16 blends showed 65-80% C12, 16-25% C14, and 4-5% C16

Method

Method/guideline:	Equivalent to OECD 474
Type:	Micronucleus Assay
GLP:	Yes
Year:	1982
Species:	Mouse
Strain:	Crl:Cd-1 (ICR) BR Swiss
Sex:	Male and female
Route of Administration:	Dermal
Concentration levels:	1000, 2500 and 5000 mg/kg. Concentrations were based on the results of a range-finding study.
Exposure period:	2 days
Statistical methods:	The group mean bodyweight was calculated for each day. The treatment and group means were compared using Student's t test. The group means and standard deviations for polychromatic erythrocytes (PCE) with micronuclei, and the group mean ratio of PCE to normochromatic erythrocytes (NCE) were calculated. Values from treated groups were compared with values from the vehicle control group using Student's t test. The test would be considered positive if there were a significant increase in micronucleated PCE at any dose level, and if a dose-related response were evident.

Test Conditions: Animals were 11 wks of age at start of treatment and weighed 28-38 g (males) and 22-30 g (females). Test article was administered undiluted. Negative control

in the test was corn oil; cyclophosphamide was positive control. Test article was applied at a maximum volume of 0.2 ml on the shaved backs of the mice of Days 1 and 2. Cyclophosphamide was given by intraperitoneal injection at a dose of 75 mg/kg. Cyclophosphamide-treated animals were sacrificed on day 3; other groups were sacrificed on days 3 and 4 and bone marrow smears were prepared. Smears were stained with May-Grunwald and Giemsa stains and examined microscopically. Approximately 1000 PCEs and all NCEs in the scan path were observed for each animal. Animals were weighed on Days 1, 3 and 4 and observed daily.

Results

Effect on PCE/NCE ratio:	Results not reported
Genotoxic effects:	Negative.
NOEL:	5.0 g/kg
Remarks:	All animals (5 per sex per group) survived to sacrifice. There were no remarkable clinical findings, or effects on body weight changes. Slides from animals given corn oil and cyclophosphamide gave expected results. Slides from animals given GULFTENE C12-16 gave no significant increase (T-test, $p< 0.05$) in micronucleated bone marrow erythrocytes or dose related response.
Reliability:	(1) Reliable without restrictions
Flag:	Key study for SIDS endpoint
References:	Gulf Life Sciences Center, Pittsburgh, Pennsylvania (1983) Micronucleus Test in Mouse Bone Marrow with GULFTENE 12-16 Administered by Dermal Application for 2 Days. Gulf Oil Chemicals Company, Sponsor (unpublished report).
Other:	This study was included in the dossier for 1-dodecene at SIAM 11. Additional information has been added.

5.8 Carcinogenicity

No data available

5.9 Reproductive Toxicity (including Fertility and Developmental Toxicity).

A. Fertility

No data available

B. Developmental Toxicity

No data available

5.10 Other Relevant Information

Aspiration

Test Substance

Identity:	C6-C18 even numbered alpha olefins

Method

Type:	General toxicity – aspiration
Species:	Rat
Strain:	Wistar
Sex:	Male
Route of Administration:	aspiration
Dose:	0.2 mL
Results:	See Remarks
Remarks:	C6-C18 alkenes (even carbon numbers, alpha olefins), source and purity unspecified, were assessed for aspiration hazard in an animal study using Wistar rats. Four or five males were used per test article. Two-tenths mL of the test material was placed in the mouths of rats that had been anesthetized to the point of apnea in a covered wide mouth gallon jar containing about 1 inch of wood shavings moistened with approximately 1 ounce of anhydrous diethyl ether. As the animals began to breathe again, the nostrils were held until the test material had been aspirated or the animal regained consciousness. All alkenes tested except 1- hexene were aspirated into the lungs. 1-Hexene was difficult to dose because of its volatility. Two animals survived because the hydrocarbon "boiled" out of the mouth before it was aspirated. All animals exposed to C_8 to C_{14} died within 24 hours. With C_{16} and C_{18}, there was only one death (C_{18}). Lung weights were increased in alkenes-treated animals compared with controls. The affected animals showed chemical pneumonitis. The report concluded that there is a significant aspiration hazard with C_6 to C_{14} alkenes.
Reference:	Gerarde, H.W. (1963) Toxicological Studies on Hydrocarbons. Archives of Environmental Health 6:329-341.
Other:	This study was included in the dossier for 1-decene at SIAM 11. Additional information has been added.

5.11 Experience with Human Exposure

No data available

6.0 References

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